RESEARCH IN THE SPACE-RELATED SCIENCES

National Aeronautics and Space Administration
Research Grant
No. NsG-518

PROGRESS REPORT

Period 1 April 1965 to 30 September 1965

UNIVERSITY OF DENVER

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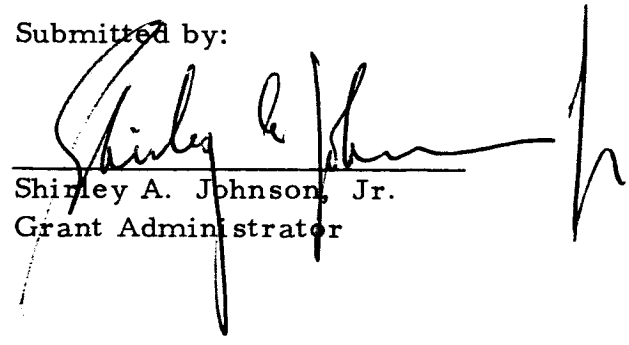
Submitted by:



Shirley A. Johnson, Jr.
Grant Administrator

Date: 15 October 1965

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Final Report, Project No. DRI-601
Final Report, Project No. DRI-604
Final Report, Project No. DRI-608
Final Report, Project No. DRI-618
Final Report, Project No. DRI-623

I. ABSTRACT

The University of Denver initiated on 1 October 1963 a significant new program of faculty and staff research in the space-related sciences under research grant NsG-518, awarded by the National Aeronautics and Space Administration. The primary purpose of this grant is to identify and support the less established, but promising investigator, as well as to foster unusual and creative thought by the allocation of limited venture funds. A total of $200,000 was vested under this grant, with $100,000 for the first year of the program and step-funded for subsequent years. After the first year of the program, supplemental funding in the amount of $150,000 was added, bringing the level of funding for the second year of the program to $125,000, and step-funded for subsequent years.

During the first twenty-four months of the program, a total of 38 requests for funding under this grant have been received. Of these, twenty-eight investigations have been supported for a total amount of $315,945; two more with requests for $64,731 are under final review, and eight have been withdrawn or rejected.

II. SUMMARY

A. Investigations Supported

Table 1 on the following page presents a summary of investigations funded during the first twenty-four months of the program.

B. Requests under Review

As of 1 October 1965, two additional requests for support are under consideration by Ad Hoc Review Committees, but no decision has yet been reached.

1. J. R. Barcus--"A Rocket-Borne Magnetometer Study of Exospheric and Wind-Induced Magnetic Variations." Funds requested--$50,579.
2. J. R. Riter--"Thermodynamic Properties of BeH_2 and BH_3 from Molecular Orbital Calculations." Funds Requested--$14,152

TABLE I

SUMMARY--INVESTIGATIONS SUPPORTED UNDER GRANT
(As of 30 September 1965)

DRI Project Number	Principal Investigator	Title of Investigation	Period of Study	Funds Allocated
601	J. A. Weese	The Theoretical Study of Three Dimensional Problems in the Classical, Linear Theory of Elasticity	22 Nov. '63 to 30 July '65	$12,301.00
602	R. Szilard (J. Moore)	A Matrix Solution of Shells of General Shape Subjected to Arbitrary Dynamic Loading	20 Dec. '63 to 15 May '65	13,310.00
603	M. T. Howerton	Mechanism of Surface Reactions--Sulfur Trioxide on Copper	23 Dec. '63 to 30 Sept. '64	4,109.00
604	M. L. Moe	Development of Adaptive System Application Criterion	30 Dec. '63 to 30 June '65	9,994.00
605	E. N. Sickafus (D. B. Barker)	The Use of Thermal Beams for Evaporation and Condensation Studies	22 Jan. '64 to 15 June '65	13,231.00
606	C. E. Lundin (M. J. Pool)	The Thermodynamics of Praseodymium-Neodymium Solid Solutions	30 Jan. '64 to 1 Jan. '65	11,598.00
607	F. H. Murcray	A Study of the Spectral Emittance of the Moon's Surface	30 Jan. '64 to 30 Jan. '65	10,562.00
608	Mueller-O'Neill	An Examination of Surface Structures Developed on Copper-Nickel Alloys by Thermal Etching in a Vacuum	1 March '64 to 31 May '65	8,365.00
609	H. Babad	Carbenoid Protonation as a Route to Carbonium Ions	1 June '64 to 31 Dec. '65	4,476.00
610	Howell-Kottenstette	Experimental Evaluation of an Improvement on a Light Gas Model Launcher	15 Feb. '64 to 1 April '64	1,810.00
611	Zeiner-Tong	Effects of 60-Day Exposure to Elevated Oxygen Tension, with Special Reference to Pulmonary Bacterial Susceptibility	1 April '64 to 30 Sept. '65	7,238.00
612	R. G. Justice	Errors Incurred in the Reduction and Mathematical Modeling of Dynamic Data	1 June '64 to 30 Nov. '65	8,475.00
613	J. R. Riter, Jr.	Potential Energy Surfaces of BeH_2 and BH_3	1 June '64 to 31 Dec. '65	12,345.00
614	J. L. Horn	Short-Period Fluctuations in Fluid Intelligence	1 June '64 to 1 Jan. '66	8,996.00
615	J. B. Calvert	Ionic Sound Waves in Plasmas	10 July '64 to 10 Jan. '66	11,235.00
616	Magee; Schmidt-Collerus	A Study of the Structure of the Transition Metal Hydryls	10 July '64 to 9 Dec. '65	12,000.00
617	A. G. Thurman	Computed Action of Pile Groups Embedded in Elastic Soils	22 July '64 to 31 March '65	1,240.00
618	A. S. West	A Survey of Available Digital Computer Procedures for Inverting and Finding the Eigenvalues and Eigenvectors of Large Matrices with Adaptations to Accommodate Current Structural Research	11 Dec. '64 to 30 June '65	3,361.00

TABLE I (continued)

DRI Project Number	Principal Investigator	Title of Investigation	Period of Study	Funds Allocated
619	J. G. Hewitt, Jr.	Electromagnetic Wave Characteristics of a Fully Ionized Gas	18 Dec. '64 to 17 Dec. '65	11,755.00
620	C. W. Chiang	Theoretical Study of Natural-Convection Flows in Closed-End Cylindrical Vessels	26 March '65 to 25 March '66	12,659.00
621	E. Tuttle	Properties of Liquid He^3 at very Low Temperatures	1 Sept. '65 to 31 Aug '66	14,570.00
622	W. D. Lansdown	Development of Circuit Design from the Logic Design of a Random Walk Machine	1 June '65 to 31 May '66	9,205.00
623	M. J. Pool	Partial Support of Proposed Research in X-ray Diffraction of Liquid Metal Systems	1 May '65 to 1 Aug '65	980.00
624	S. H. Carpenter	Dislocation Damping in LiH	1 July '65 to 30 June '67	26,773.00
625	E. N. Sickafus	Surface Spikes as a Mode of Crystal Growth & Overseas Travel Expense	1 June '65 to 31 May '66	38,119.00
626	R. Szilard	Matrix Solution of Shells of Arbitrary Shape Subjected to Arbitrary Dynamic Loading	20 July '65 to 20 March '66	11,900.00
627	G. Mallett	Microstrain, Stacking Fault, & Atomic Displacement Determinations	15 Sept. '65 to 15 March '67	22,840.00
628	J. A. Young	Fluoride Ion Reactions of Fluorocarbon Derivitives	1 Jan. '66 to 31 Dec. '66	12,498.00

III. BUDGET

A. Expenditures on Supported Investigations

Table II below presents a summary of funds committed to the twenty-eight investigations supported to date, showing expenditures during the first twenty-four months of the program as well as the funds committed for subsequent expenditure.

TABLE II

FUNDS ALLOCATED AND FUNDS EXPENDED
(As of 30 September 1965)

DRI Project Number	Principal Investigator	Period of Investigation	Total Funds Granted	Funds Expended 10/1/63-9/30/65	Committed Funds to be Expended after 10/1/65
601	J. A. Weese	Nov. '63-July '65	12,301	12,301	0
602	R. Szilard	Dec. '63-May '65	13,310	13,310	0
603	M. T. Howerton	Dec. '63-Sept. '64	4,109	4,109	0
604	M. Moe	Dec. '63-April '65	9,994	9,994	0
605	E. Sickafus	Jan. '64-June '65	13,231	13,231	0
606	C. Lundin	Jan. '64-Jan. '65	11,598	11,598	0
607	F. Murcray	Jan. '64-Jan. '65	10,562	10,562	0
608	Mueller-O'Neill	Mar. '64-May '65	8,365	8,365	0
609	H. Babad	June '64-Jan. '66	4,476	4,476	0
610	W. Howell	Feb. '64-April '64	1,810	1,810	0
611	Tong-Zeiner	April '64-Sept. '65	7,238	7,238	0
612	G. Justice	June '64-Nov. '65	8.475	7,545	930
613	J. Riter	June '64-Dec. '65	12,345	12,710	(365)
614	J. Horn	June '64-Jan. '66	8,996	9,020	(24)
615	J. Calvert	July '64-Jan. '65	11,235	9,172	2,063
616	Magee; Schmidt-Collerus	July '64-Dec. '65	12,000	7,593	4,407
617	A. Thurman	July '64-Mar. '65	1,240	1,240	0
618	A. West	Dec. '64-June '65	3,361	3,361	0
619	Hewitt-Boone	Dec. '64-Dec. '65	11,755	7,173	4,582
620	Chiang	Mar. '65-Mar. '66	12,659	2,207	10,452
621	Tuttle	Sept. '65-Aug. '66	14,570	692	13,878
622	Lansdown	June '65-May '66	9,205	5,577	3,628
623	Pool	May '65-Aug '65	980	980	0
624	Carpenter	July '65-June '67	26,773	5,034	21,739
625	Sickafus	June '65-May '66	38,119	21,577	16,542
626	Szilard	July '65-March '66	11,900	2,269	9,631
627	Mallett	Sept. '65-March '67	22.840	7,726	15.114
628	Young	Jan. '66-Dec. '66	12,498	0	12,498
		Subtotal	$315,945	$200,870	$115,075
		Publication Costs	1,465	1,465	0
		Total	$317,410	$202.335	$115,075

B. Summary of Funds Expended (1 October 1963 to 30 September 1965):

Table III below presents a summary, by category, of the funds expended during the first twenty-four months of the program.

TABLE III

FUNDS EXPENDED
(10/1/63 through 9/30/65)

Labor (including Fringe Benefits and Stipends)	$120,076.06
Supplies	16,383.28
Travel	3,530.05
Equipment	28,235.97
Overhead	34,109.83
Total	$202,335.19

IV. ADMINISTRATION OF THE GRANT

The "procedures" for the administration of this grant were reported in the 12 May 1964, first semi-annual report submitted to the National Aeronautics and Space Administration.

V. RESEARCH INVESTIGATIONS UNDER SUPPORT

1. PROJECT NO. DRI-601

Principal Investigator: Dr. John A. Weese, Research Engineer and Associate Professor of Mechanical Engineering

Title of Investigation: The Theoretical Study of Three Dimensional Problems in the Classical, Linear Theory of Elasticity

Funds Allocated: $12,301.00

Period of Study: 22 November 1963 to 30 July 1965*

ABSTRACT:

This study is concerned with the analytical methods of solving three-dimensional problems in the classical linear theory of linear elasticity with particular emphasis upon obtaining useful numerical results from theoretical investigations. With rare exception, the solutions to such problems must be expressed as infinite, or even double infinite, series. Often the rate of convergence of the series solution is so slow that, from a practical point of view, it is impossible to obtain numerical results which would be of use to a designer.

This convergence problem is being approached through the solution of two problems, each in a different curvilinear coordinate system. These problems are:

1) A Torus Rotating about the Axis of Symmetry (Toroidal Coordinates).

2) A Half-Space Containing a Heated Spherical Cavity. (Bispherical Coordinates).

The solutions to these two technically significant problems appear to be obtainable within the period of this investigation. The solution of either problem will clear the way for the treatment of other problems of interest in its coordinate system.

*Extended from 21 November 1964.

FINAL REPORT:

A final report summarizing this investigation is presented in Appendix A.

STATUS OF EXPENDITURES:

Funds Granted	$12,301.00
Funds Expended	12,301.00
Funds Remaining	$ 0.00

2. PROJECT NO. DRI-602

Principal Investigator: Dr. Rudolph Szilard, Senior Research Engineer and Professor, Department of Civil Engineering
Jay Moore and Anita West--Co-investigators

Title of Investigation: A Matrix Solution of Shells of General Shape Subjected to Arbitrary Dynamic Loading

Funds Allocated: $13,310.00

Period of Study: 20 December 1963 to 15 May 1965

ABSTRACT:

The purpose of this investigation is to develop a matrix method of analysis for the solution of shells of general shape and with arbitrary boundary conditions subjected to arbitrary dynamic loading. Primary emphasis is placed on obtaining a mathematical model for the "dis-assembled" structure and on determining the stiffness coefficient of such structural element.

Triangular double curved shells have been chosen as individual elements which when assembled and the corresponding stiffness matrices when compiled are able to represent any shell surface. The matrix inversion of the compiled stiffness matrix yields the flexibility matrix of the whole system. The solution of eigenvalue problem of the flexibility matrix gives the natural frequencies and natural modes of the free vibration of the arbitrary shells. Fourier series techniques will be used in connection with the arbitrary dynamic load describing the forced part of the vibration.

PROGRESS REPORT:

This research investigation has received an extension to continue it for a second year. The progress report concerning this study is presented under the successor grant, DRI-626.

STATUS OF EXPENDITURES:

Funds Granted	$13,310.00
Funds Expended	13,310.00
Funds Remaining	$ 0.00

3. PROJECT NO. DRI-603

Principal Investigator:	Dr. M. T. Howerton, Professor of Chemical Engineering
Title of Investigation:	Mechanism of Surface Reactions--Sulfur Trioxide on Copper
Funds Allocated:	$4,109.00
Period of Study:	23 December 1963 to 30 September 1964

ABSTRACT:

The formation of surface films at gas-solid interfaces has been investigated by a fluorescent X-ray emission technique. Initial studies were made with sulfur trioxide and copper. The investigation has been extended to include surface films at the hydrogen sulfide-copper and hydrogen selenide-copper interfaces.

Sulfur and copper X-ray emission intensities have been measured as a function of exposure time over a range of temperatures and gas pressures. The gas pressure over the interface ranged from 0.1 mm Hg. to 500 mm Hg.; the surface temperature ranged from 100°C to 180°C. The intensity measurements have been converted to molar ratios of sulfur to copper by means of intensity calibrations made with pure CuS, Cu_2S and known deposits of sulfur on copper surfaces. The molar ratio of S/Cu has been correlated as a function of time by means of a two-parameter equation having the form

$$S/Cu = [\ (a - 2b)\ (1 - e^{-a\theta}\ ) + a(1 - e^{-b\theta}\ )\ ]\ /4\,(a - b)$$

The parameters a and b are functions of the vapor density and surface temperature. This equation predicts that the maximum S/Cu ratio at time infinity would be 0.5.

FINAL REPORT:

The final report on this investigation appeared in the 31 March 1965, Semi-Annual Progress Report.

STATUS OF EXPENDITURES:

Funds Granted	$4,109.00
Funds Expended	4,109.00
Funds Remaining	$ 0.00

4. PROJECT NO. DRI-604

Principal Investigator:	Dr. Maynard L. Moe, Research Engineer and Assistant Professor of Electrical Engineering
Title of Investigation:	Development of Adaptive System Application Criterion
Funds Allocated:	$9,994.00
Period of Study:	30 December 1963 to 30 June 1965*

ABSTRACT:

The basic objective of this study is the development of a quantitative design criterion which can be used to determine when an adaptive system is needed to control a plant with varying parameters. The study deviates from the apparent direction of current research in adaptive feedback systems, and, if successful, the procedures developed could affect the basic notion of what constitutes a good design in the synthesis of feedback control systems.

FINAL REPORT:

A final report summarizing this investigation is presented in Appendix A.

STATUS OF EXPENDITURES:

Funds Granted	$9,994.00
Funds Expended	9,994.00
Funds Remaining	$ 0.00

*Extended from 30 November 1964

5. PROJECT NO. DRI-605

Principal Investigator:	Dr. E.N. Sickafus, Research Physicist and Associate Professor of Physics D. Boyd Barker, Collaborator
Title of Investigation:	The Use of Thermal Beams for Evaporation and Condensation Studies
Funds Allocated:	$13,231.00
Period of Study:	22 January 1964 to 15 June 1965.*

ABSTRACT:

Two experimental techniques are under investigation which, when developed, will extend the state-of-the-art in solid-vapor interface studies. The first consists of the development of an ultrasensitive mass determination method, for use in a high vacuum system, coupled with a suspended oven and/or a suspended collector to be used for measuring the vapor pressures in the region of 1 torr and at high temperatures (~700°C). The second involves the development of thermal beam procedures for studying condensation kinetics while allowing only one degree of translational freedom in the vapor-solid interaction.

FINAL REPORT:

The final report on this investigation appeared in the 31 March 1965, Semi-Annual Progress Report.

STATUS OF EXPENDITURES:

Funds Granted	$13,231.00
Funds Expended	13,231.00
Funds Remaining	$ 0.00

*Extended from 21 January 1965.

6. PROJECT NO. DRI-606

Principal Investigator:	Charles E. Lundin, Senior Research Metallurgist Dr. Monte J. Pool, Consultant
Title of Investigation:	The Thermodynamics of Praseodymium-Neodymium Solid Solutions
Funds Allocated:	$11,598.00
Period of Study:	30 January 1964 to 1 January 1965

ABSTRACT:

It is the intent of this study to establish the heats of mixing of alloys of the binary rare earth system, praseodymium, neodymium. The technique used is liquid-tin solution calorimetry. The heats of solution of the pure components in tin will be determined. The heats of solution of the alloys in tin will be determined. From these data the heats of mixing will be established. A plot of the heat of mixing versus composition will be made, and the conformity to solution ideality will be determined.

FINAL REPORT:

The final report on this investigation appeared in the 31 March 1965, Semi-Annual Progress Report.

STATUS OF EXPENDITURES:

Funds Granted	$11,598.00
Funds Expended	11,598.00
Funds Remaining	$ 0.00

7. PROJECT NO. DRI-607

Principal Investigator:	Frank H. Murcray, Research Physicist
Title of Investigation:	A Study of the Spectral Emittance of the Moon's Surface
Funds Allocated:	$10,562.00
Period of Study:	30 January 1964 to 30 January 1965*

ABSTRACT:

The absence of a region of low emissivity in lunar emission spectra has been cited, in support of the dust layer hypothesis, as indicating that siliceous rocks are absent from the lunar surface.

Critical examination of the existing data shows that it lacks the accuracy required to eliminate the possiblity of existence of a significant percentage of exposed siliceous rocks on the lunar surface. The existing spectra indicate that the moon's surface cannot be entirely composed of siliceous rocks in unmodified form but more sensitive measurements are required before the percentage of the lunar surface, which may be composed of these rocks, can be fixed closer than a range from 0 to 40%.

The recent measurements of lunar albedo in the near infrared from Stratoscope II strongly indicate that the assumption of an emissivity near unity at the longer wavelengths should not be accepted without conclusive evidence.

The intention of this investigation is to accurately determine the emissivity of the lunar surface as a function of wavelength from 8.0μ to 12.0μ with a spectral resolution greater than .1μ. Spectral measurements will be much more sensitive to a small percentage of exposed rock than previous measurements which integrated a wide spectral interval.

FINAL REPORT:

The final report on this investigation appeared in the 31 March 1965, Semi-Annual Progress Report.

*Extended from 30 September 1964

STATUS OF EXPENDITURES:

Funds Granted	$10,562.00
Funds Expended	10,562.00
Funds Remaining	$ 0.00

8. PROJECT NO. DRI-608

Principal Investigators:	Dr. William M. Mueller Professor of Metallurgy Dennis O'Neill, Co-principal Investigator and Research Metallurgist
Title of Investigation:	An Examination of Surface Structures Developed on Copper-Nickel Alloys by Thermal Etching in a Vacuum
Funds Allocated:	$8,365.00
Period of Study:	1 March 1964 to 31 May 1965*

ABSTRACT:

The surface structures that result from heating copper-nickel alloys in a vacuum environment are being examined by electron microscopy techniques. The observed changes in surface structure with variations in temperature and composition will be correlated with available data on thermal etching in an effort to elucidate some of the present gaps in the field of thermal etching.

FINAL REPORT:

A final report summarizing this investigation is presented in Appendix A.

STATUS OF EXPENDITURES:

Funds Granted	$8,365.00
Funds Expended	8,365.00
Funds Remaining	$ 0.00

*Extended from 28 February 1965.

9. PROJECT NO. DRI-609

Principal Investigator:	Dr. Harry Babad, Assistant Professor of Chemistry
Title of Investigation:	Carbenoid Protonation as a Route to Carbonium Ions
Funds Allocated:	$4,476.00
Period of Study:	1 June 1964 to 31 December 1965

ABSTRACT:

The properties of high energy cations, prepared by carbenoid protonation,will be studied to correlate leaving group and solvent characteristics to cationic reactivity. The syntheses of a series on monocyclic olefins containing a side chain carboxaldehyde will be undertaken, and these model compounds will be subject to conversion to cationic intermediates, via the tosylhydrazone pyrolysis reaction. The degree and stereospecificity of the pi cyclization reaction will be the criteria of cationic reactivity.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

We are at present in the final stages of our preliminary survey of the reaction of p-toluenesulfonylhydrazine derivatives as routes to high energy intermediates. Progress has been made in three areas, and pending the receipt of final analytical data, some of this work will be submitted for publication.

The results of the aprotic and protonic decomposition of the p-toluenesulfonylhydrazine (PTSH) derivative of 4,4-dimethyl-2,5-cyclohexadienone were perhaps the least satisfying of our studies. In either solvent system, only a low percent (less than 5%) of volatile materials of a complex nature were obtained, the principal products being ditoluenesulfone and p-azeotoluene. These products were similar to those obtained by A. J. Fry[1] recently from the decomposition of the PTSH derivative of 4-methyl-4-trichloromethyl-2,5-cyclohexadienone, and leave unanswered the question of the nature of the in situ rearrangement of dienone carbenes at high temperatures.

[1] A. J. Fry, J. Am. Chem. Soc., 87 1816 (1965).

We have almost completed the separation of the complex mixtures obtained in the protonic (ten components) and aprotic (seven components) decomposition of the PTSH derivative of Δ3-cyclohexenecarboxaldehyde with the aid of an Aerograph A-700P chromatograph.[2] Analysis shows the following compounds (C_7H_{10}) to be present in varying amounts: Cyclohepta-1, 4-diene, cyclohepta-1, 3-diene, bicyclo(4. 1. 0)heptene-2, bicyclo(4. 1. 0)heptene-2, as well as several C_7 cyclohexadienes and two compounds that have been tentatively identified as norbornene and one of the unsaturated bicyclo(3. 2. 0)heptenes. Further purifications of these materials, quantitative hydrogenation, as well as spectral analysis (IR, UV and NMR) should confirm the structures of the remaining components. This will allow us to elucidate the reaction paths taken by the carbenoin and carbonium ion intermediates in this series of compounds.

In a search for straight-forward route to the unsaturated aldehydes* from commercially available carboxylic acids, we explored the possibility of applying the McFadeyn-Stevens Reaction to the synthesis of aliphatic aldehydes. This reaction has been used successfully to prepare aromatic aldehydes from the PTSH derivatives of carboxylic acid chlorides related to benzoic acid, but had not resulted in the formation of aldehydes from aliphatic acid chlorides. The PTSH derivatives of n-butyric acid, i-butyric acid and cyclohexanecarboxylic acid were decomposed under protonic conditions in ethylene glycol containing an excess of dissolved sodium to give the corresponding aldehydes in fair yields. The aldehydes were identified as their 2-4 DNP derivatives, as well as by spectrographic means. In addition to these aldehydes there remain two major unidentified components in the reaction mixtures which are <u>not</u> butyric acid or the 1, 3-dioxalone (from ethyleneglycol and the aldehyde) which are presently under investigation.

The preceding results bear out our premise that solvent composition and reaction "contact time" plays an important role in the decomposition of PTSH derivatives leading to high energy intermediates. More work is being planned in this area in order to examine some of the many unsolved problems that remain. The author would like to express his thanks to Barbara Dahl, James B. Wood, Arthur Stiles and Washington Herbert without whom this research would not have been possible.

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[2] Purchased with funds obtained from the National Science Foundation Institutional Instructional Scientific Equipment Grant GE-9031.

* necessary to our pyrolysis studies

STATUS OF EXPENDITURES:

Funds Granted	$4,476.00
Funds Expended	4,476.00
Funds Remaining	$ 0.00

10. PROJECT NO. DRI-610

Principal Investigators: William G. Howell, Research Engineer, and James P. Kottenstette, Research Engineer

Title of Investigation: Experimental Evaluation of an Improvement on a Light Gas Model Launcher

Funds Allocated: $1,810.00

Period of Study: 15 February 1964 to 1 April 1964

ABSTRACT:

The objective of this study was to experimentally evaluate a proposed new technique for improving the performance of a light gas model launcher. The technique to be evaluated involved the following changes in the pumping sequence:

1) Change the loading conditions to assure that the pump tube piston reaches the ends of its stroke with a relatively high velocity.

2) Accelerate a secondary piston into the launch tube by conversion of the kinetic energy stored in the pump tube piston at the end of its stroke.

This process should maintain a higher average pressure on the base of the model (or sabot) being launched and a higher velocity should result.

FINAL REPORT:

The final report on this investigation appeared in the 12 May 1964, Semi-Annual Progress Report.

STATUS OF EXPENDITURES:

Funds Granted	$1,810.00
Funds Expended	1,810.00
Funds Remaining	$ 0.00

11. PROJECT NO. DRI-611

Principal Investigators: Dr. F. N. Zeiner, Professor of Zoology
Dr. J. L. Tong, Associate Professor of Bacteriology

Title of Investigation: Effects of 60-Day Exposure to Elevated Oxygen Tension, with Special Reference to Pulmonary Bacterial Susceptibility

Funds Allocated: $7,238.00

Period of Study: 1 April 1964 to 30 September 1965

ABSTRACT:

The work has a double purpose. It (1) continues studies of this laboratory on the ability of laboratory animals to withstand elevated 0_2 tensions for 60-day periods and (2) it explores the possibility of after-effects of such exposure following return to normal atmospheric conditions.

The animals are divided into experimental and control groups. The experimental group is subjected to an essentially pure 0_2 atmosphere at reduced barometric pressure. The control group is maintained under identical housing conditions, but supplied with air at ambient pressure. Samples of lung tissue for microscopic examination are obtained from each group immediately following the 60-day exposure. The remaining animals of each group are tested for pulmonary tuberculosis susceptibility by controlled bacterial aerosol exposure, this being the challenge following return to normal atmospheric conditions.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

1) Exposures of female mice of the CD strain for 60-day periods to artificial atmospheres were completed. Survival rate on all runs was very near 100%. Lungs have been examined for indications of oxygen poisoning.

2) Animals of all groups have been challenged for susceptibility to pulmonary tuberculosis. Tests utilizing the density of

lungs to determine degree of infection have been completed and data have been analyzed statistically.

3) The lungs are being examined visually by a panel of pathologists to determine degree of infection. This phase is near completion and the final report will include comparisons of results from the different methods of analysis that have been used.

The cooperation of Lt. Col. W. C. Morse of the Research and Development Laboratory, Microbiology, Fitzsimons General Hospital, is gratefully acknowledged.

STATUS OF EXPENDITURES:

Funds Granted	$7,238.00
Funds Expended	7,238.00
Funds Remaining	$ 0.00

12. PROJECT NO. DRI-612

Principal Investigator:	Dr. R. Gailor Justice, Assistant Professor of Chemical Engineering
Title of Investigation:	Errors Incurred in the Reduction and Mathematical Modeling of Dynamic Data
Funds Allocated:	$8,475.00
Period of Study:	1 June 1964 to 30 November 1965*

ABSTRACT:

This project concerns a study of the propagation of measurement errors in the reduction of dynamic data. Its basic goal is to obtain some insight into the most efficient and sensitive procedure for data reduction. The variables to be examined are domain in which mathematical modeling is to be done, the least squares arguments utilized and procedures for data adjustments. The effect of these variables will be evaluated by variance tests. These variances will be calculated from differences in experimental data and model data obtained as a function of the aforementioned variables.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

All data runs have been processed in the time domain using the convolution integral. The data were processed in the raw form (unnormalized) and in two modified forms with the input and the output data normalized in separate tests. It was found that there was no difference in the parameters obtained with the normalized data. That is, it does not seem to matter whether the input or the output data were normalized. This is probably due to the fact that the convolution integral is a linear operator. There was a significant difference, however, in the Peclet number parameter between the normalized and unnormalized data. This difference did not appear until the material balance was off some 10-15%. Also the speed of convergence was much slower with the unnormalized data.

*Extended from 1 June 1965.

The effective length to average velocity ratio did not seem to vary between the normalized and unnormalized data.

The numerical Fourier transforms and the numerical LaPlace transforms have been obtained for all runs. These transforms exhibit no nonlinearities. These transforms are being correlated to those obtained from the mathematical model; however, sufficient data has not yet been obtained to make a comparison between the parameters obtained in this manner and those obtained using the convolution integral.

STATUS OF EXPENDITURES:

Funds Granted	$8,475.00
Funds Expended	7,545.00
Funds Remaining	$ 930.00

13. PROJECT NO. DRI-613

Principal Investigator:	Dr. John R. Riter, Jr., Assistant Professor of Chemistry
Title of Investigation:	Potential Energy Surfaces of BeH_2 and BH_3
Funds Allocated:	$12,345.00
Period of Study:	1 June 1964 to 31 December 1965

ABSTRACT:

Experimental thermodynamic data for many transitory species of interest in chemistry are completely lacking or at best meager and inconclusive. For polyatomic molecules the computation of these properties by the methods of quantum mechanics has not been done with anything approaching the amount of effort put forth on diatomics by, for example, the groups at the University of Chicago and IBM's San Jose Laboratory.

Two of the simplest polyatomics are BeH_2 and BH_3. We will compute their heats of formation as accurately as possible using a simple basis set of Slater-type orbitals with the self-consistent field energy error, the correlation energy, and the relativistic energy all estimated from i) isoelectronic systems and ii) the hydrides LiH and CH_4. The fundamental vibration frequencies will be estimated from those of the diatomic fragments and from other molecules with similar geometries. Simple valence bond and hybridization considerations predict a linear symmetric BeH_2 ($D_{\infty h}$) and a planar BH_3 (D_{3h}). This work should yield good estimates of the two unique internuclear distances, one for each molecule. A rather complete set of thermodynamic functions will then be calculated in the rigid-rotor harmonic-oscillator approximation. The computed heat of formation of BeH_2 will hopefully shed some light on an interesting chemical problem; the decomposition of solid beryllium hydride etherate upon warming.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

Our B5500 program to compute the energy of BeH_2 as a function of geometry, in the SCF approximation per the Roothaan scheme, is in the final stages and awaits only the empircal determination of the three-center integrals as a function of geometry themselves before we can

determine the LCAO-SCF energy. We believe this can be accomplished by the first of the year. It was found necessary to go to the IBM machines with these programs for the three- and four-center integrals; an attempt to translate the Fortran tape into Algol failed. We have used the B5500 for the bulk of our work however.

The molecular correlation energies for BeH_2 and BH_3 have been estimated as 0.177 and 0.259 atomic units respectively, with relativistic corrections of 0.002 and 0.005 atomic units. The third decimal is the limit of our confidence, but since 0.001 atomic unit is about 0.6 kcal/mol we feel we can obtain chemically useful information. The third and last correction term is more difficult to treat though not as large as the correlation energy. We have done and are doing computations on isoelectronic systems with the same number of closed shells and subshells and feel we will soon have established a rational extrapolation procedure. The computed LCAO-SCF energy when combined with the three correction terms above will give the best estimate of total energy from which the heats of formation follow immediately.

Earlier plans to evaluate the force constants analytically as the second potential energy-normal coordinate derivative were rather rudely upset by work done this past year with Professor Paul Phillipson of the University of Colorado Physics Department. Using rather accurate approximate wave functions for the hydrogen molecule and molecular-ion we found the force constant to be extremely sensitive to the nonlinear parameters in the wave functions. Since variation of the orbital exponents with molecular geometry for a polyatomic is far beyond our capabilities, we will settle for the still realistic approach of estimating fundamental frequencies from those of diatomic fragments and other hydrides as well as linear symmetric and planar symmetric molecules. On the other hand our LCAO results should yield reliable estimates of the equilibrium Be-H and B-H distances.

STATUS OF EXPENDITURES:

Funds Granted	$12,345.00
Funds Expended	12,710.00
Funds Remaining	$ (365.00)

14. PROJECT NO. DRI-614

Principal Investigator:	Dr. John L. Horn, Assistant Professor, Department of Psychology
Title of Investigation:	Short-period Fluctuations in Fluid Intelligence
Funds Allocated:	$8,996.00
Period of Study:	1 June 1964 to 1 January 1966*

ABSTRACT:

This study will examine empirically the hypothesis that a complex human ability known as "fluid intelligence" fluctuates over periods as short as a few hours or days. Parallel forms of tests known to measure this factor will first be constructed. Using these tests repeated measurements will be obtained over 20 occasions on a sample of 100 male adults, thus generating a 20 × 40 × 100 "box" data. This "box" will be analysed by newly developed multivariate methods in an effort to isolate reliable changes in abilities over occasions.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

Test construction has been completed. Tests have been administered and are now being scored. Computer analyses have been laid out and will be carried out shortly.

STATUS OF EXPENDITURES:

Funds Granted	$8,996.00
Funds Expended	9,020.00
Funds Remaining	$ (24.00)

*Extended from 1 June 1965

15. PROJECT NO. DRI-615

Principal Investigator:	Dr. James B. Calvert, Research Physicist and Assistant Professor of Physics
Title of Investigation:	Ionic Sound Waves in Plasmas
Funds Allocated:	$11,235.00
Period of Study:	10 July 1964 to 10 January 1966

ABSTRACT:

The purpose of this study is to investigate the generation and propagation of ion-acoustic waves in a weak plasma, and the interaction of these waves with ordinary acoustic waves. The study includes both experimental and theoretical aspects.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

The apparatus for generating the plasma consists of a plasma tube and an associated ultra-high vacuum system for evacuating, cleaning, and filling the tube.

The plasma tube is of pyrex glass, approximately 80 mm. in diameter and 300 mm. long, fitted with a nickel anode wire and a stainless steel cathode. Two cathode designs are to be investigated. One is a plain flat plate, the other a similar plate fitted with about 900 sharp needles 30 mm. long. The direct-current power supply is a Harrison Laboratories type 6522A, providing 0-2 kv. at 0-100 ma.

The ultra-high vacuum system consists of a Consolidated Vacuum Corporation type GF-25 three-stage water-cooled oil diffusion pump with a polyphenyl ether working fluid, a type TSG-52 zeolite sorbent trap, two Granville-Phillips type C valves, a Varian type UHV 12-P Bayard-Alpert gauge, and a quartz-tube Helium leak designed in this laboratory. These components are connected by 1/2-inch diameter pyrex tubing and are mounted within a bake-out oven (except for the diffusion pump).

The acoustic tube, which is about 50 mm. in diameter and 200 mm. long, is a pyrex tube designed to be fused into the sides of the plasma tube with the tube axes at right angles. This tube contains an iron diaphragm 25 mm. in diameter and 0.05 mm. thick at one end, and a diode electron-mobility microphone converted from a type 15-E triode at the other. Because it was necessary to attach the diaphragm with soft solder to avoid warping, this tube is not capable of high-temperature bake-out. Means to eliminate this difficulty are being studied. Associated equipment consists of a power supply and control circuit for the diode, two 20-db. voltage gain amplifiers, an oscilloscope for signal display, a pulse generator, and a diaphragm driver converted from an earphone receiver.

The above apparatus has been assembled and is being tested.

The initial experiments will be the measurement of sound velocity in the acoustic tube by the pulse-delay method, and the maintenance of a quiet, uniform discharge in the plasma tube. The operating pressure is expected to be about 2 torr in ultra-pure Helium. This operating pressure will be measured by using the Bayard-Alpert gauge filament as a Pirani gauge, using another gauge filament as a reference. A special Wheatstone bridge circuit has been constructed for this measurement.

STATUS OF EXPENDITURES:

Funds Granted	$11,235.00
Funds Expended	9,172.00
Funds Remaining	$ 2,063.00

16. PROJECT NO. DRI-616

Principal Investigators:	Dr. Charles B. Magee, Research Metallurgist and Associate Professor of Metallurgy; and Dr. Josef J. Schmidt-Collerus, Senior Research Chemist and Associate Professor of Chemistry
Title of Investigation:	A Study of the Structure of the Transition Metal Hydryls
Funds Allocated:	$12,000.00
Period of Study:	10 July 1964 to 9 December 1965*

ABSTRACT:

The purpose of this study is to investigate the molecular and crystalline structures of the transition metal hydryls. These compounds, of apparent stoichiometries $M(LiH)_4$ and $MH(LiH)_4$ (M represents a transition metal), have been synthesized with rhodium and iridium. The techniques being used to investigate the structures are infrared absorption spectrum analysis, X-ray diffraction analysis, and nuclear magnetic resonance spectrum analysis.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

As stated in the previous progress report, the mull technique for obtaining infrared spectra of solids was found not to give reproducible or interpretable results when applied to the hydryl compounds. We then turned to thin films deposited on KBr plates for obtaining infrared absorption spectra. It was found possible to obtain very thin films of LiH and LiD by evaporating these materials under vacuum. The absorption bands obtained using these films reproduced the bands reported by others for these materials.

During the last few months many attempts have been made to obtain thin films of the hydryls by the evaporation technique. By rapidly heating $(LiH)_4Rh$ or $(LiD)_4Rh$ in a tantalum boat in vacuum, thin

*Extended from 9 June 1965

films are formed on plates suspended over the boat. These films show infrared absorption bands: for $(LiH)_4Rh$ a single band is observed at about 430 cm^{-1} and for $(LiD)_4Rh$ two bands are observed at about 420 and 440 cm^{-1}. However, these bands cannot be attributed to the hydryl compounds. In one experiment with $(LiH)_4Rh$ the film was analyzed for rhodium by means of X-ray flouresence; no rhodium was found in the film. The tantalum boat from which the material was evaporated likewise was analyzed and was found to contain rhodium. Thus it must be concluded that these materials decompose during evaporation.

It might be expected that $(LiH)_4Rh$ would decompose to form LiH and Rh, and that the film obtained would be made up of LiH. This is not the case, however, because LiH absorbs at about 590 cm^{-1} while the band observed for the film is at 430 cm^{-1}. Our conclusion at the moment is that the hydryl decomposes to H_2, Li, and Rh and that a lithium film is formed. This film then reacts with the constituents of air, despite attempts to prevent exposure to air, to form the oxide, the hydroxide, and/or the carbonate. This conclusion is based on the fact that when lithium metal itself is evaporated the film shows a band at about 430 cm^{-1}.

We have not given up hope of evaporating the hydryls without decomposition. We feel that if we can flash evaporate the liquid hydryl rather than the solid we will have a better chance of getting the whole molecule into the vapor phase. We are planning to carry out experiments along these lines.

Another approach to obtaining infrared spectra of these materials has been tried during this report period. We have attempted to find a solvent for $(LiH)_4Rh$. The following non-aqueous solvents were tried: ethanol, diethyl ether, trichloroethylene, acetone, methyl alcohol, benzene, hexane, dimethyl formamide, and carbon disulfide. Carbolic acid (phenol in water) was also tried. None of these solvents readily dissolved the hydryl. In the case of ethanol there was evidence of slight dissolution or reaction but the infrared spectrum showed no bands other than those of ethanol. With diethyl ether the liquid slowly turned yellow indicating, probably, that a reaction was taking place. With carbolic acid the liquid slowly turned red, again indicating reaction. Although the possibilities are not completely exhausted, it appears that these materials are going to resist going into any kind of solution.

STATUS OF EXPENDITURES:

Funds Granted	$12,000.00
Funds Expended	7,593.00
Funds Remaining	$ 4,407.00

17. PROJECT NO. DRI-617

Principal Investigator:	Dr. Allen G. Thurman, Assistant Professor of Civil Engineering
Title of Investigation:	Computed Action of Pile Groups Embedded in Elastic Soils
Funds Allocated:	$1,240.00
Period of Study:	22 July 1964 to 31 March 1965*

ABSTRACT:

This project was to continue previous studies on the analytical prediction of pile performance based upon the type of piles used and upon the soil conditions as determined by standard tests. In particular, methods of developing the research to a broad scope, including pile groups and methods of sponsoring research at this broad scope, were to be investigated.

FINAL REPORT:

The final report on this investigation appeared in the 31 March 1965, Semi-Annual Progress Report.

STATUS OF EXPENDITURES:

Funds Granted	$1,240.00
Funds Expended	1,240.00
Funds Remaining	$ 0.00

*Extended from 21 January 1965

18. PROJECT NO. DRI-618

Principal Investigator:	Anita S. West Research Mathematician
Title of Investigation:	A Survey of Available Digital Computer Procedures for Inverting and Finding the Eigenvalues and Eigenvectors of Large Matrices with Adaptations to Accommodate Current Structural Research
Funds Allocated:	$3,361.00
Period of Study:	11 December 1964 to 30 June 1965

ABSTRACT:

The partial differential equations of motion of shell structures subject to arbitrary loads may be extremely difficult or even impossible to solve. Since the digital computer is now an available tool for the structural engineer, current research has been directed towards methods which involve matrix formulation of large systems of algebraic equations and matrix solutions for discrete elements, and these require rapid and accurate computer solutions. Recognizing the accuracy problems inherent in working with large matrices, this study has been undertaken to survey the available computer programs for large matrix inversions and for eigenvalue and -vector solutions; to check out these programs and translate, where necessary, for the Burroughs B5500 computer, thus providing a handbook of program input information and at the same time providing techniques for using these programs most efficiently, with a minimum of effort on the part of the researcher.

FINAL REPORT:

A final report summarizing this investigation is presented in Appendix A.

STATUS OF EXPENDITURES:

Funds Granted	$3,361.00
Funds Expended	3,361.00
Funds Remaining	$ 0.00

19. PROJECT NO. DRI-619

Principal Investigator:	Dr. Jack G. Hewitt, Jr., Assistant Professor Electrical Engineering and Research Engineer
Title of Investigation:	Electromagnetic Wave Characteristics of a Fully Ionized Gas
Funds Allocated:	$11,755.00
Period of Study:	18 December 1964 to 17 December 1965

ABSTRACT:

We are examining, both theoretically and experimentally, the electromagnetic wave properties of a highly ionized plasma.

Theoretically, we are developing tensor expressions for the impedance matrix and propagation constant. From these terms we can interpret the nature of a plane wave interacting with the plasma. The spatial arrangement of the electromagnetic energy coupled into the plasma will be developed from the energy equation and the electromagnetic stress tensor.

Experimentally, we are checking the above theory by propagating a plane wave through a highly ionized magnetic cesium plasma and measuring attenuation, reflection and phase shift relative to air. These results are related to the known thermodynamic properties of the plasma.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

During this period, the experimental apparatus has been virtually completed. The vacuum system has been assembled and is performing normally. The plasma tube has been received and the electrode assembly has been constructed and placed in the tube.

The X-band microwave interferrometer has been assembled and its performance checked by inserting dielectrics between the horns in a position which will be subsequently occupied by the plasma.

The vacuum system is currently being outgassed in order to achieve an ultrahigh vacuum prior to generating the plasma.

In view of the large amount of theoretical work already done with respect to small amplitude wave interactions we have been able to devote our effort primarily to the irregularities (zeros and resonances). We are investigating coupling modes at the plasma resonant and gyro frequencies in an effort to understand the mode conversion processes in the presence of a static magnetic field.

STATUS OF EXPENDITURES:

Funds Granted	$11,755.00
Funds Expended	7,173.00
Funds Remaining	$ 4,582.00

20. PROJECT NO. DRI-620

Principal Investigator:	Dr. C. W. Chiang, Research Engineer and Associate Professor of Mechanical Engineering
Title of Investigation:	Theoretical Study of Natural-Convection Flows in Closed-End Cylindrical Vessels
Funds Allocated:	$12,659.00
Period of Study:	26 March 1965 to 25 March 1966

ABSTRACT:

This study is concerned with the analytical solutions of natural-convection flows in closed-end cylindrical vessels with particular emphasis being placed upon obtaining exact solutions of temperature and velocity profiles in the laminar flow regime. Solutions for a transient condition are the ultimate purpose of this study.

The technique used to solve the problem is to modify the one used by H. Blasius and E. Pohlhausen when they obtained exact solutions of the laminar boundary-layer equations for a flat plate. The partial differential equations of continuity, momentum and energy expressed in cylindrical coordinates for an imcompressible fluid are transformed into ordinary differential ones by introducing a lumped variable as a function of displacement and time. A stream function as a power series of the lumped variable is introduced. Exact solutions can be obtained by the use of boundary conditions.

PROGRESS REPORT (Period 1 April 1965 to 30 September 1965):

Since the investigator devoted almost his whole summer to another project there is not much of significance to report at this time. However, an initial effort has been made during April and September to investigate the transformation of partial differential equations into ordinary differential equations for transient conditions. Some progress has been reached.

STATUS OF EXPENDITURES:

Funds Granted	$12,659.00
Funds Expended	2,207.00
Funds Remaining	$10,452.00

21. PROJECT NO. DRI-621

Principal Investigator:	Dr. Elizabeth R. Tuttle, Asst. Professor of Physics and Research Physicist
Title of Investigation:	Properties of Liquid He^3 at Very Low Temperatures
Funds Allocated:	$14,570.00
Period of Study:	1 September 1965 to 31 August 1966

ABSTRACT:

Calculations of the energy per particle at zero temperature in liquid He^3, which will have been begun in the summer of 1965, will be completed. An investigation of the microscopic theory of a Fermi liquid at very low but finite temperatures will be made, and the necessary modifications of the Landau phenomenological theory of a Fermi liquid, as determined by the results of the above investigation, will be made also. The thermodynamic properties (specific heat, energy per particle, chemical potential) of liquid He^3 at very low temperatures will then be calculated.

PROGRESS REPORT (Period 1 September 1965 to 30 September 1965):

The zero temperature calculations begun at the beginning of the summer are progressing slowly; the main difficulty encountered seems to be loss of significant figures. We believe that this can be circumvented by the use of double-precision in the computer program. At present, these calculations are being pursued on the IBM 709 at the University of Colorado.

The terms obtained through second order in the reaction matrix expansion of the microscopic theory for finite temperature have been obtained; and expressions for the energy per particle, free energy, entropy, quasiparticle energy, and momentum distribution have been derived. The outlines of a phenomenological theory in agreement with the microscopic theory have been drawn, but several of the details are not yet clear.

STATUS OF EXPENDITURES:

Funds Granted	$14,570.00
Funds Expended	692.00
Funds Remaining	$13,878.00

22. PROJECT NO. DRI-622

Principal Investigator:	Dr. William D. Lansdown, Asst. Professor of Electrical Engineering
Title of Investigation:	Development of the Circuit Design from the Logic Design of a Random Walk Machine
Funds Allocated:	$9, 205. 00
Period of Study:	1 June 1965 to 31 May 1966

ABSTRACT:

A search of commercially available logic units has revealed two nearly equal lines that are appreciably better than other lines considered. The line that seems somewhat more satisfactory is the Fairchild CTμL 952-957 line. The cost of logic integrated circuits using this family is $18, 800, and a crude estimate on the overall cost of components of the random walk machine is $36, 000.

The transformation from the logic to the circuit design is largely completed using the Fairchild line.

The likelihood of obtaining a Department of Electrical Engineering experimental computer has temporarily delayed design of the interface and control procedure for the controlling computer.

Data for writing a proposal(s) have been compiled and should be available in one or two months.

PROGRESS REPORT (Period 1 June 1965 to 30 September 1965):

1. Choice of commercially available logic

A search of commercially available logic integrated circuits (IC's) has been made. The following figure of merit was used as a criteria:

$$f = CD$$

C is the cost of one bit of a circular, left and right shifting shift register. D is the average delay of the bit in nanoseconds, and is inversely proportional to the operating speed. The function f is to be minimized. The two best results are tabulated below:

Line of Logic	C	D	f
Motorola MC 351-361	$13.00	22	286
Fairchild CTμL 952-957	16.07	18	290

The Fairchild line requires 2 1/3 IC's per bit and the Motorola 4 IC's per bit. The Fairchild units thus require fewer innerconnections and simpler circuit boards.

The logic for the random walk machine using the Fairchild IC's will cost $18,800 which allows 10% margin. No consideration has yet been made for the cost of the circuit board, connectors, wiring, controls, power supplies, random bit unit, cabinet for housing and miscellaneous hardware. Continued studies will be made to estimate these costs more accurately, but a crude estimate places the cost of the components of the random walk machine at $36,000.

2. Transformation of Circuit Design

As implied above, the circuit design of the random walk machine is largely completed on the basis of the Fairchild IC's. The Fairchild units use AND and NOT units and the OR function is accomplished by connecting the outputs of the AND's. Thus the circuit design is virtually a direct replacement of the AND-OR-NOT logic design. The Motorola units, which are NAND units (using negative logic), would require somewhat more transformation of the logic from the AND-OR-NOT form.

3. Design of Innerface and Control Procedure

Because of the likelihood of the Dept. of Electrical Engineering obtaining its own computer of the GE 4000 PAC family, the design of the innerface and control procedure for the B 5500 computer has been postponed till later in the study. It would be much more convenient to use a department experimental computer rather than the machine servicing the entire University. Work on this phase will be performed later in the project.

4. Writing of Proposal

Data for writing proposals have been compiled and should be available in one or two months. Proposals will be submitted to national foundations to obtain support for building the random walk machine.

STATUS OF EXPENDITURES:

Funds Granted	$9,205.00
Funds Expended	5,577.00
Funds Remaining	$3,628.00

23. PROJECT NO. DRI-623

Principal Investigator:	Dr. Monte J. Pool, Asst. Professor of Metallurgy and Research Metallurgist
Title of Investigation:	Partial Support of Proposed Research in X-ray Diffraction of Liquid Metal Systems
Funds Allocated:	$980.00
Period of Study:	1 May 1965 to 1 August 1965

ABSTRACT:

To determine to a greater extent the experimental difficulties which possibly may be associated with research on "X-ray Diffraction Studies of Liquid Tin Alloys," it is deemed judicious to discuss X-ray diffraction techniques of liquid metal systems with several of the leading authorities in the field.

FINAL REPORT:

A final report summarizing this investigation is found in Appendix A.

STATUS OF EXPENDITURES:

Funds Granted	$980.00
Funds Expended	980.00
Funds Remaining	0.00

24. PROJECT NO. DRI-624

Principal Investigator: Dr. Steve H. Carpenter, Research Associate

Title of Investigation: Dislocation Damping in LiF

Funds Allocated: $26, 773. 00

Period of Study: 1 July 1965 to 30 June 1967

ABSTRACT:

Dislocation dynamics, i. e., dislocation motion and mobility, are being investigated on different glide planes in single crystal LiF. The basis for this investigation comes from the fact that, although crystals of LiF much prefer to glide on {110} planes, they can be forced to glide on {100} planes by means of a suitable stress distribution. This plastic anisotropy is of particular interest, since elementary criteria predict that {100} should be the preferred glide plane in LiF. Because the mechanism determining glide in any particular plane is intimately related to the ability of dislocations to move and to the amount of dislocation motion in that particular glide plane, it is believed that an investigation of this nature will help provide an understanding of this anomaly.

Internal friction (also known as dislocation damping) measurements will be the method used to determine the dislocation dynamics. Measurements will be made in the kilocycle frequency range using a piezoelectric composite oscillator. This method is extremely well suited for this investigation. By measuring the damping of a properly oriented sample in a longitudinal vibrational mode, it is possible to determine the dislocation motion on one set of glide planes. Then by measuring the damping of the same sample in a torsional vibrational mode, it is possible to determine the dislocation motion in the other glide plane.

PROGRESS REPORT: (Period 1 July 1965 to 30 September 1965):

Work on the project has been initiated and is progressing. The necessary electronic equipment has been purchased and received. High purity single crystal LiF samples have been obtained from the Harshaw Chemical Co. An apparatus has been constructed which allows

for the internal friction or damping to be measured as a function of strain amplitude in the range $\epsilon = 10^{-4}$ to 10^{-8}. The apparatus consists essentially of a piezoelectrically driven composite oscillator. The basis of the apparatus consists of two straight α quartz crystals cemented end to end. The crystals have been cut and matched in length for a resonant frequency of 50.0 kilocycles/second. Gold electrodes have been deposited on the quartz crystals as a means of obtaining an electric field in the quartz. Vibrations at the resonant frequency are obtained by applying an A. C. electric signal to the electrodes of one of the quartz crystals, called the driver crystal. The other quartz crystal, called the gauge, develops an alternating voltage between its electrodes which is used as a measure of the strain amplitude. Preliminary damping data has been taken for dislocation motion on the {110} glide planes. The constants of the system have been characterized and evaluated.

Construction is presently in progress on an apparatus to measure the damping as a function of temperature. Upon completion this apparatus will provide the capability to measure the damping in the temperature range of room temperature to the melting point.

STATUS OF EXPENDITURES:

Funds Granted	$26,773.00
Funds Expended	5,034.00
Funds Remaining	$21,739.00

25. PROJECT NO. DRI-625

Principal Investigator:	Dr. E. N. Sickafus, Associate Professor of Physics and Research Physicist
Title of Investigation:	Surface Spikes as a Mode of Crystal Growth
Funds Allocated:	$38,119.00
Period of Study:	1 June 1965 to 31 May 1966

ABSTRACT:

A new mode of crystal growth has been observed during the sublimation of $NiBr_2$. This growth takes the form of surface spikes and leads to localized growth rates that are greater than that to be expected from the Burton, Cabrera, and Frank theory. The mechanism for the nucleation of this spike growth is not understood and it is for this purpose that the present program of research has been initiated. Experiments conducted to date indicate that the mechanism of nucleation will necessitate a much lower than ordinary free energy for the growing species. This is indicated by the appearance of droplets with the surface spikes and the development of these spikes at 500 degrees centigrade below the normal melting point. The experiments being conducted under this program are designed to investigate the means by which the necessary lowering of free energy is obtained.

PROGRESS REPORT (Period 1 June 1965 to 30 September 1965):

The following experiments have been designed to investigate the mechanism for the lowering of the free energy of $NiBr_2$ that is associated with the development of surface spikes: (1) Mass spectrographic analysis of the diffusion species that accompany the vaporization of $NiBr_2$ from Knudsen cells constructed from different materials, (2) in situ growth studies to characterize the development of the spikes, and (3) surface analysis by electron microprobe techniques.

1) Impurity Studies (Mass Spectrographic Analysis)

As initially designed, the basic impurity study will involve an analysis of the vapor from heated samples of $NiBr_2$. $NiBr_2$ samples

from various sources will be heated in Knudsen cells in contact with nickel, glass, porcelain and quartz in an attempt to separate impurities initially in the $NiBr_2$ from those possibly introduced by the materials used to construct the crystal-growth chambers. The vapor will be analyzed by a Residual Gas Analyzer (Veeco Model GA-4) which is a specialized form of 60°, magnetic-separation mass spectrometer. A partial pressure of 10^{-12} torr can be detected in the mass range of 2-300. With reduced sensitivity the mass range from 12 to 300 can be scanned in 0.1 second to monitor transient vapor evolution during cell warmup.

The vacuum system available for this study is constructed of 4 & 6 inch diameter Pyrex pipe sections blanked off with brass end plates which are sealed with neoprene "O" rings. The 4-inch oil diffusion pump can be trapped at either CO_2 or liquid N_2 temperatures. A pressure of $2\text{-}3(10^{-6})$ torr can be obtained with reasonable pumping times. Several runs were made with commercial K&K $NiBr_2$ in a nickel Knudsen cell located 10 inches from a port in an end plate to which the RGA was attached by a 10 inch, 1 inch diameter tubulation. Traces of Fe and Mn were detected (confirming earlier Electron Microprobe runs) but the lack of peaks for Br and HBr indicated that much vapor was probably being trapped before reaching the RGA. A new Knudsen cell furnace has been constructed and the mounting arrangement changed to put the cell orifice only about 3 inches from the RGA ionization chamber. After furnace bakeout and a thorough analysis of background vapors in the system, a new series of sample runs will be initiated.

2) In situ Growth Studies

A very simple vycor growth chamber has been designed which incorporates a window of electrically conducting glass. The electrically conducting glass window will serve as a substrate for growth and will offer the ability of controlling the temperature of the substrate through the heat dissipation of the current passing through the glass. A prototype has been constructed but problems have been encountered due to differences in differential thermal expansion of the materials of the growth chamber and the window.

3) Electron Microprobe Studies

Preliminary arrangements have been made to use an electron microprobe to investigate variations in the chemical concentration of

the surface of the $NiBr_2$ crystals and the droplets on the surface. Previous work of this kind has revealed the presence of manganese, copper, cobalt, and iron impurities in the droplets.

Two supplemental fundings were granted to this program after it was initiated. The first was in the amount of $500, to assist in travel to the Summer School in Electron Microscopy of Thin Crystals at Cambridge, England in July. This study covered the theory of image formation by lattice defects using both the kinematical and dynamical treatments. With this background, it will be possible to employ new experimental techniques to investigate the structural geometry of surface spike growth both by X-ray imaging and electron imaging techniques. To expedite these new studies a second supplement was received in the amount of $21,382. These monies are for the purpose of purchasing X-ray Microfocus equipment and Lang camera accessories. With this equipment the Lang method and double crystal method of X-ray imaging of defects will be employed in studies of the defect state of layered structure crystals such as $NiBr_2$.

STATUS OF EXPENDITURES:

Funds Granted	$38,119.00
Funds Expended	21,577.00
Funds Remaining	$16,542.00

26. PROJECT NO. DRI-626 (Extension of DRI-602)

Principal Investigators: Dr. Rudolph Szilard,
Professor, Civil Engineering
and Sr. Research Engineer

Title of Investigation: A Matrix Solution of Shells of Arbitrary Shape Subjected to Arbitrary Dynamic Loading

Funds Allocated: $11,900.00

Period of Study: 20 July 1965 to 20 March 1966

ABSTRACT:

An improved discrete element approach is used in the solution of the problem. For discrete elements, rectangular plate elements have been selected considering membrane and bending theories with a provision for supplementary consideration of the curvature effects. The "node"-points where continuity is expressed are located at the center of the fixed edges. The elements of the stiffness-matrix of the discrete shell-element are determined by subjecting the "node"-points to unit translations and rotations. The statically equivalent forces and moments acting at the nodal points, which are produced by the unit motions, are determined by solving the differential equations of the plate and two-dimensional stress problems, respectively. The supplementary effect of the curvature is expressed by a fictitious lateral loading. In solution of the differential equations, finite difference methods have been utilized, which allows extended use of computers. The stiffness matrix of the total structure is obtained by compiling the individual stiffness matrices of the disassembled structure. Any physically possible boundary condition including cut-outs, variation of shell thickness can be considered by simple modification of the stiffness matrix of the total structure. The static and dynamic shell problems are formulated in matrix form suitable for computer analysis. The arbitrary variation of the load in space is treated by replacing of the loads by equivalent concentrated loads acting at the node points. The time dependency of the dynamic loads are expressed in Fourier series. The accuracy of the method is compared with known "exact" solutions.

PROGRESS REPORT: (Period 20 July 1965 to 30 September 1965)

This project is the continuation of the terminated DRI project 602, which resulted in the determination of the stiffness matrices of rectangular plate elements subjected to unit motion which were not in the plane of the element representing the bending theory of shell.

The stiffness factors corresponding to the membrane theory of shells have been obtained by introducing in-plane unit motions at the node points. The results have been checked by solving plate and two-dimensional stress problems for which analytical solutions are available. Good agreement and rapid convergence has been achieved in the case of plate problems; this is reported in the paper entitled "Static and Dynamic Analysis of Plates of Arbitrary Shape and Boundary Condition" (Szilard and Hubka) scheduled for publication in the 1965 Proceedings of the International Association for Bridge and Structural Engineering. The accuracy of the solution of two-dimensional stress problems (±11% with relatively coarse subdivision) has been reported in the paper entitled "A Matrix and Computer Solution of Cylindrical Shells of Arbitrary Shape" (Szilard) at the International Symposium on Shell Structures held recently in Budapest, Hungary. Investigation of the convergence of the membrane solution, including the improvements of the coefficients, are presently under study. The possibility of complete automation of the solution is also under investigation.

STATUS OF EXPENDITURES:

Funds Granted	$11,900.00
Funds Expended	2,269.00
Funds Remaining	$ 9,631.00

27. PROJECT NO. DRI-627

Principal Investigator:	Gavin Mallett, Chief X-ray Diffraction Center and Research Metallurgist
Title of Investigation:	Microstrain, Stacking-Fault, and Atomic Displacement Determinations
Funds Allocated:	$22,840.00
Period of Study:	15 September 1965 to 15 March 1967

ABSTRACT:

This research project will undertake the development of a computer program for the evaluation of microstrains, stacking-fault probabilities and atomic displacements from X-ray diffraction data of polycrystalline materials. Techniques employing X-ray diffraction are feasible for these evaluations; however, the high degree of accuracy necessary requires the application of elaborate correction factors to intensity data not ordinarily used in conventional diffraction methods.

The ultimate objective of the program will be to study these phenomena in nonstoichiometric or intermetallic compounds and terminal solid solutions. The program will be developed initially on a theoretical basis and then applied to specific real material for modification to insure reliability and accuracy in further extensive analyses. The association of microstrains and atomic imperfections with material properties presents a wide field of potential research in the development of ultra-high strength materials.

PROGRESS REPORT (15 September 1965 through 30 September 1965):

The Picker Radiation Electronic Analyzer, authorized by NASA for purchase under this grant, has been ordered. As this grant was initiated only two weeks ago, there is nothing of further significance to report at this time.

STATUS OF EXPENDITURES:

Funds Granted	$22,840.00
Funds Expended	7,726.00
Funds Remaining	$15,114.00

28. PROJECT NO. DRI-628

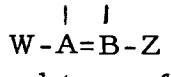
Principal Investigator:	Dr. J. A. Young, Senior Research Chemist
Title Of Investigation:	Fluoride Ion Reactions of Fluorocarbon Derivatives
Funds Allocated:	$12,498.00
Period of Study:	1 January 1966 to 31 December 1966

ABSTRACT:

Alkali metal fluorides have been found to bring about a surprising variety of reactions of fluorocarbons and their derivatives. These reactions have been utilized rather empirically and fundamental knowledge concerning steric and electronic effects is very scanty.

The objectives of this proposal are twofold; the first is to delineate the necessary requirements of molecular structure for the occurrence of fluoride ion catalysis, and the second is to synthesize molecules of new and unusual structure, particularly those containing novel bond types.

The first objective will be carried out by varying in stepwise fashion the atoms of groups surrounding the reactive center



and observing the effects of such variation on extent, rate, and type of reaction.

The second objective will be carried out by investigating reactions of unusual perfluoro nucleophiles which may lead to fluorocarbon derivatives in which sulfur, nitrogen, phosphorus or oxygen atoms are bonded to carbon or nitrogen.

PROGRESS REPORT:

Project does not begin until 1 January 1966.

STATUS OF EXPENDITURES:

Funds Granted	$12, 498. 00
Funds Expended	0. 00
Funds Remaining	$12, 498. 00

APPENDIX A

Final Report, Project No. DRI-601

Final Report, Project No. DRI-604

Final Report, Project No. DRI-608

Final Report, Project No. DRI-618

Final Report, Project No. DRI-623

FINAL REPORT

THE THEORETICAL STUDY OF THREE DIMENSIONAL PROBLEMS IN THE CLASSICAL, LINEAR THEORY OF ELASTICITY

A Research Project Supported by a NASA
Grant in the Space Related Sciences

NsG - 518

Project No. DRI - 601

University of Denver

July 1965

SUBMITTED BY:

J. A. Weese
Principal Investigator
Department of Mechanical Engineering

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I. SUMMARY

The purpose of this study was to further the capability of treating three dimensional problems in the classical theory of linear elasticity, particularly those problems which are axially symmetric. With rare exception, the solutions to these problems must be expressed as infinite series. In certain instances, notably in spherical coordinates (see e.g. [1]), the rate of convergence of the resulting series can be studied directly since analytical expressions for the coefficients in the terms of the series can be obtained. In other curvilinear coordinate systems, however, the coefficients are given as the solution vector to an infinite set of linear algebraic equations resulting from the boundary conditions and the behavior of the coefficients can only be inferred by solving successively larger subsets of the infinite set of equations. Since it is often impossibly difficult to formulate an elasticity problem in any coordinate system other than the one for which the coordinate surfaces conform to the boundaries of the body, it is important to investigate methods for improving convergence in other coordinate systems.

It was proposed to study the problem of convergence in two specific problems in different, but related, coordinate systems, the problems were:

1. A Torus Rotating about the Axis of Symmetry (Toroidal Coordinates)
2. A Half Space Containing a Heated Spherical Cavity (Bispherical Coordinates).

The application of digital computer programming techniques is essential to obtain meaningful results. This investigator, believing that detailed knowledge of programming methods is required by the analyst, undertook the task of educating himself to the point of requiring little outside programming assistance. This has been found not only to result in better, more flexible programs but also a computer oriented analyst finds ways to shorten the analysis considerably. Several tedious stages of the analysis were eliminated by programming the computer to perform certain classes of algebraic manipulations. These developments will make it possible to attempt more advanced problems for which certain phases of the analysis would become prohibitively difficult.

Because of the mutual interest with Dr. William E. Warren of the Sandia Corporation, the problem of determining the state of stress in a half space containing a heated spherical cavity was undertaken

first. Some preliminary work had actually been done on the particular solution of this problem before the award of this contract and it was felt that this analysis should be continued.

The solution to the problem of a heated spherical cavity in a half space consists of constructing a particular solution which removes the temperature dependent terms from the displacement equation and finding a complementary solution which satisfies the homogeneous displacement equation and annihilates the stresses of the boundary. As originally planned, the complementary solution was to be an improved version of one developed by this investigator in his doctoral thesis [2] and Dr. Warren was to supply the particular solution.

Both solutions can only be obtained as infinite series. In addition, the particular solution depends upon the temperature distribution which is also an infinite series. To obtain the coefficients in either solution it is necessary to solve an infinite set of algebraic equations. This is done by truncating the set of equations and observing the changes in the calculated values of the coefficients as successively more terms are used.

When Dr. Warren's first attempt at the particular solution gave series expansions which appeared to diverge, he discovered a method of employing redundant solutions which gave a solution which could be truncated with known error. The improvement was so striking that it led to the hope that similar operations on the complementary solution would solve its convergance problems also.

Since a method by which the complementary solution could be truncated with known error would constitute a significant advanced in elasticity theory, it was immediately decided to test it. A complete discussion of the redundant solution method is contained in the section by that title. Suffice it to say here that after a great deal of effort consuming much of the alloted time, the method failed. The effort was not entirely in vain, however, because a great deal was learned about the nature of solutions in the bispherical coordinate system and which properties of them are likely to be important. Unfortunately, insufficient time and funds remained to complete the solution of the problem in the contract. As a result of this study, however, and a review entitled "The Use of Bispherical Coordinates to Analyze Three-Dimensional Stress Concentrations in the Theory of Elasticity," a contract was obtained from the Sandia Corporation to complete this problem and some others closely related to it.

In the course of the study, it was necessary to reexamine an earlier publication by Sternberg and Sadowsky [3]. This work was done without the aid of digital computer facilities and consequently only very limited numerical results were presented. During this study results were extended and a brief note is being submitted for publication in the Journal of Applied Mechanics. It is entitled "Numerical Results for the Axisymmetric Problem of an Infinite Region Containing Two Spherical Cavities of Equal Size."

Although the problem of a torus rotating about the axis of symmetry remained untouched, the detailed study of the properties of solutions in bispherical coordinates pointed out some features which are likely to be the cause of trouble with an earlier analysis performed by this investigator and Dr. T. P. Mitchell of Cornell University. In particular, an alternate form of the axisymmetric solution was found which may well be the key to that problem. A master's candidate became interested in the problem and elected to determine experimentally the stresses in a rotating torus for his thesis work. Project funds were used to have the torus machined for his experiment which is not likely to be completed before January 1966.

II. FORMULATION OF THE THERMOELASTIC PROBLEM

Prescribed axisymmetric temperature or heat flux distributions are applied to the surface of the spherical cavity and the plane boundary of the semi-infinite, isotropic, linearly elastic solid shown in Figure 1. The resulting stress field is to be determined for steady state temperature distribution with ambient temperature at infinity under the conditions that the material constants are independent of temperature and the boundaries are stress free.

In rectangular coordinates x_i, the steady state temperature field is governed by the Fourier heat conduction equation which, written in Cartesian tensor form, is

$$T_{,ii} = 0 \tag{1}$$

In the theory of uncoupled thermoelasticity the displacements are governed by the equation [4]

$$(1 - 2\nu)u_{i,kk} + u_{k,ki} = 2(1 + \nu)\,\underline{\alpha}\,T_{,i} \tag{2}$$

Where the u_i are the displacement components, ν is Poisson's ration, and $\underline{\alpha}$ is the coefficient of thermal expansion. From the stress strain relations

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{3}$$

and the generalized Hook's law for an isotropic body

$$\sigma_{ij} = \frac{2\nu}{1-2\nu}\,G\delta_{ij}\epsilon_{kk} + 2G\epsilon_{ij} - \frac{E\,\underline{\alpha}\,T}{1-2\nu}\,\delta_{ij} \tag{4}$$

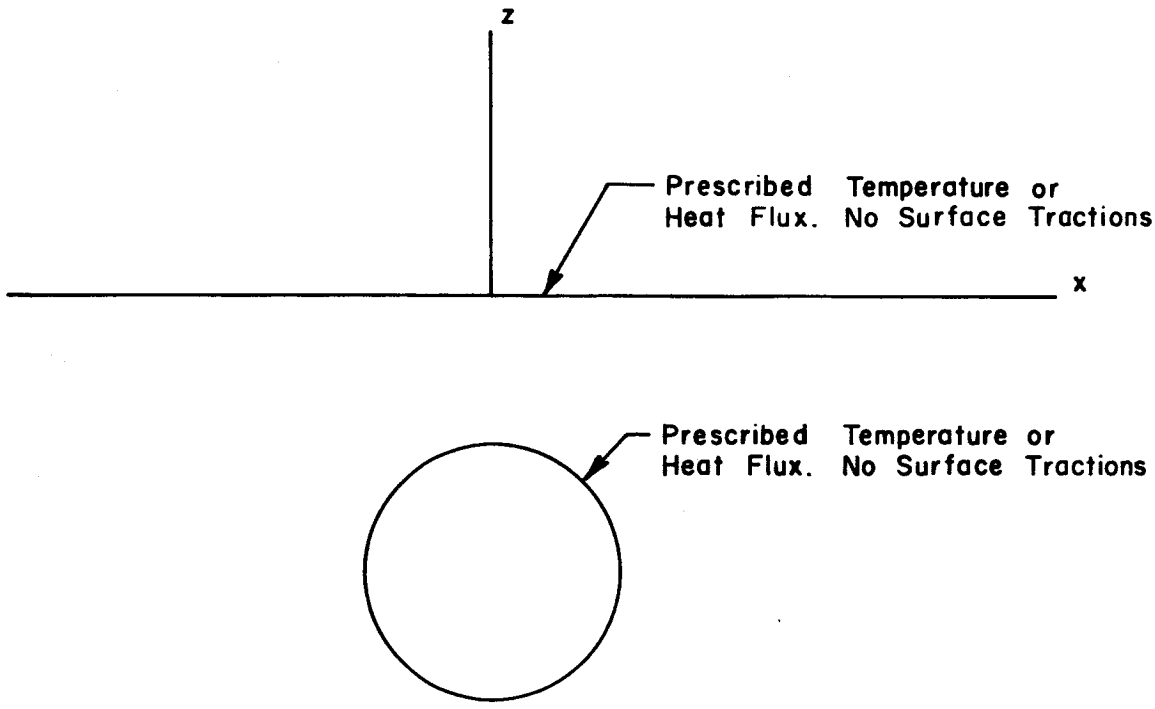
the stresses can be written as

$$\sigma_{ij} = G\left\{u_{i,j} + u_{j,i} + \frac{2}{1-2\nu}\left[\nu u_{k,k} - (1+\nu)\,\underline{\alpha}\,T\right]\delta_{ij}\right\} \tag{5}$$

Where G is the shear modulus of the material and δ_{ij} is the Kronecker delta.

The bispherical coordinate system, given by the transformation equations

$$x = a\frac{\sin\beta}{\cosh\alpha - \cos\beta}\cos\gamma,\quad y = a\frac{\sin\beta}{\cosh\alpha - \cos\beta}\sin\gamma,$$
$$z = -a\frac{\sinh\alpha}{\cosh\alpha - \cos\beta} \tag{6}$$



Temperature and Stresses at Infinity to be Zero.

Figure 1.

is well suited for this problem since the coordinate surfaces $\alpha = \alpha_0$ are spheres of radius $a|\text{csch}\,\alpha_0|$ with centers at $(0, 0, -a\coth\alpha_0)$. As shown in Figure 2 the surface $\alpha = 0$ is the plane $z = 0$ plus a sphere of infinite radius. The poles at $z = \mp a$ correspond to $\alpha = \pm\infty$. The surfaces $\beta = \beta_0$ are formed by the rotation about the z-axis of the $x \geq 0$ part of a circle in the x-z plane whose radius is $a\csc\beta_0$ and whose center is at $x = a\cot\beta_0$, $z = 0$. These surfaces pass through the two poles. The coordinate surface $\gamma = \gamma_0$ is a meridinal half plane. As indicated in the figure by the right angle intersection of the coordinate surfaces, the bispherical coordinate system is orthogonal. The constant a is merely a scale factor.

For convenience the following notation will be used throughout the rest of the report

$$\begin{aligned} p &= \cos\beta & q &= \cosh\alpha \\ \bar{p} &= \sin\beta & \bar{q} &= \sinh\alpha \end{aligned} \tag{7}$$

Since the problem is axisymmetric the temperature, stress and displacement fields must be independent of γ and the stresses $\sigma_{\alpha\gamma}$ and $\sigma_{\beta\gamma}$ must be zero. The condition of axial symmetry is implicit in all that follows unless stated otherwise.

The boundary conditions required for a unique solution to the thermoelastic problem may be expressed as

$$\left.\begin{aligned} T(0,p) \text{ or } \left[\frac{q-p}{a}\frac{\partial T}{\partial\alpha}\right]\Bigg|_{\alpha=0} &= f_0(p) \\ T(\alpha_c,p) \text{ or } \left[\frac{q-p}{a}\frac{\partial T}{\partial\alpha}\right]\Bigg|_{\alpha=\alpha_c} &= f_c,(p) \end{aligned}\right\} \tag{8}$$

$$\left.\begin{aligned} \sigma_{\alpha\alpha}(0,p) = \sigma_{\alpha\beta}(0,p) &= 0 \\ \sigma_{\alpha\alpha}(\alpha_c,p) = \sigma_{\alpha\beta}(\alpha_c,p) &= 0 \end{aligned}\right\} \tag{9}$$

where α_c is the value of α on the cavity.

The analysis proceeds with a solution to the heat equation (1) with the boundary conditions (8) which yields the temperature distribution in the body. Once the temperature distribution has been established the

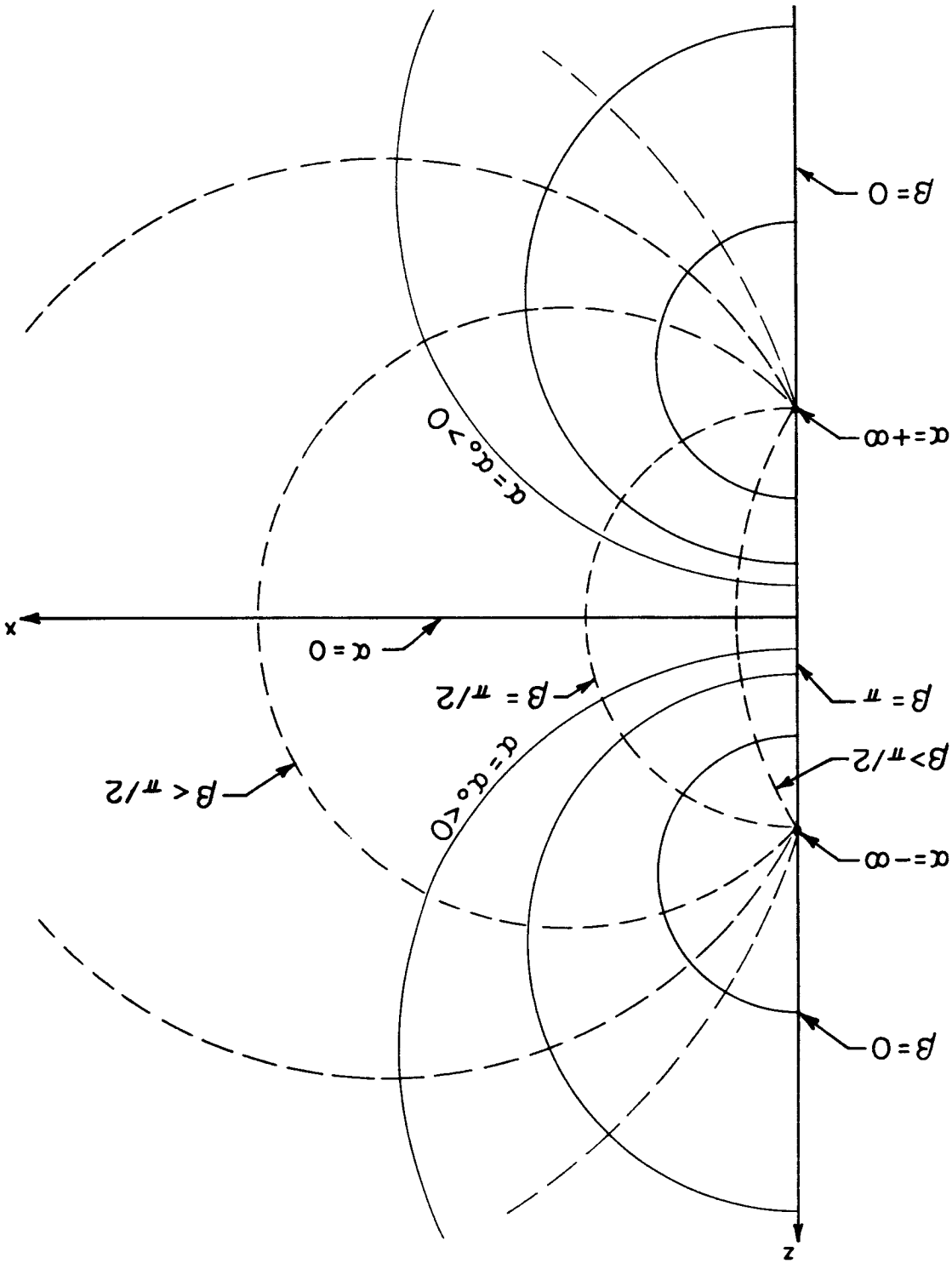


Figure 2. The Bispherical Coordinate System

solution of the displacement equation (2) is obtained as the sum of a particular integral given by a thermoelastic potential and a general solution of the homogeneous form of (2) in terms of the Boussineq-Papkovich potentials. Constants in the series expansions in the Boussinesq-Papkovich potentials are evaluated from the stress free boundary conditions (9).

III. THE TEMPERATURE DISTRIBUTION AND THE PARTICULAR SOLUTION*

The steady state axisymmetric temperature distribution must satisfy Laplace's equation (1). As discussed in [5] the required function in bispherical coordinates is

$$T = \mu \sum_{n=0}^{\infty} \{ T_n^0 \, C_n(\alpha) + T_n^1 S_n(\alpha)\} P_n(p) \tag{10}$$

where

$$\mu = (q-p)^{\frac{1}{2}} \qquad C_n(\alpha) = \cosh \frac{1}{2} k\alpha$$

$$k = 2n + 1 \qquad S_n(\alpha) = \sinh \frac{1}{2} k\alpha$$

T_n^0 and T_n^1 are constants and $P_n(p)$ is the Legendre polynomial of degree n and argument p. The constants T_n^0 and T_n^1 are determined from the boundary condition (8). It is, therefore, necessary to expand the functions

$$f_0(p)/(1-p)^{\frac{1}{2}} \qquad \text{and} \qquad f_c(p)/(q_c-p)^{\frac{1}{2}}$$

in Fourier-Legendre series. This is greatly facilitated by use of the relation

$$(q-p)^{-\frac{1}{2}}\Big|_{\alpha=\alpha_i} = \sqrt{2} \sum_{0}^{\infty} e^{-\frac{k}{2}|\alpha_i|} P_n(p) \tag{11}$$

which is derived from the generating function for Legendre polynomials, see [5]. If, as is often the case, $f_0(p)$ and $f_1(p)$ are polynomials, equation (11) is used along with repeated application of the recurrence formula for Legendre polynomials, see e.g. [6],

---

* As mentioned earlier, most of the work on the particular solution was done originally by Dr. William E. Warren of the Sandia Corporation and subsequently checked by this investigator. Portions of this section have been adapted from a draft written by Dr. Warren of the paper which will be authored jointly and submitted for publication. The material is included in this report for clarity and continuity and is being done with Dr. Warren's consent.

$$(2n+1)\, p\, P_n(p) = (n+1)P_{n+1}(p) + nP_{n-1}(p) \tag{12}$$

The simplest example is that of constant temperature T_c on the surface of the cavity and zero temperature on the plane $a = 0$ and at infinity. For zero temperature on the plane, the T_n^0 must be zero for all n. For constant temperature on the surface of the cavity $f_1(p)$ is T_c and consequently from (10) and (8)

$$T_n^1 = \sqrt{2}\, T_c \frac{e^{-\frac{1}{2}k a_c}}{S_n(a_c)} \tag{13}$$

The condition of zero temperature on the plane and constant heat input on the surface of the cavity, H_c, is more complicated in that it leads to the infinite set of equations

$$\begin{aligned} &-nT_{n-1}^1 C_{n-1}(a_c) + [\overline{q}_c S_n(a_c) + (2n+1) q_c C_n(a_c)]\, T_n^1 \\ &-(n+1)T_{n+1}^1 C_{n+1}(a_c) = 2\sqrt{2}\, a \frac{H_c}{K}\, e^{-\frac{1}{2}k a_c} \qquad (n=0, 1, 2\ldots) \end{aligned} \tag{14}$$

where K is the coefficient of thermal conductivity. Fortunately this set of infinite equations converges very rapidly and the constants T_n^1 can readily be determined on a computer.

With the temperature distribution established it is possible to remove the temperature dependent terms from the displacement equation and the stress strain equation by a thermoelastic potential defined by the equations

$$2Gu_i = \Phi_{,i} \tag{15}$$

where

$$\Phi_{,ii} = 2\left(\frac{1+\nu}{1-\nu}\right) G \underline{a}\, T \tag{16}$$

For the steady state temperature conditions considered here it follows from (1) that T must be harmonic and, therefore, Φ must be biharmonic or

$$\Phi_{,iijj} = 0 \tag{17}$$

The biharmonic function Φ may be expressed on terms of harmonic functions X and Ω as

$$\Phi = r^2 X + z\, \Omega \tag{18}$$

equations is not only valid (i.e. nonsingular) but after a few manipulations of adding and subtracting equations, the coefficient matrix is triangularized and the coefficients can readily be obtained by back substitution.

However, if either of the harmonic functions X or Ω of (18) is taken to be zero, corresponding to the vanishing of the K_n^0 and K_n^1 or L_n^0 and L_n^1, then the two sets of equations (21) yield an apparently divergent series representation of Φ. This is contrasted with the above case which provides a method of finding a particular solution which corresponds exactly to the temperature series truncated at a finite number of terms. Consequently, the appropriateness of the particular solution is keyed to the temperature distribution, the series for which converges quite rapidly. In many instances three place accuracy is achieved if the T_n^1 are taken to be zero for all $n \geq 3$.

The stress field arising from the thermoelastic potential Φ and the temperature T is obtained by transforming the Cartesian stress components given in (5) directly into the bispherical coordinate system.

$$
\begin{aligned}
a^2\sigma_{\alpha\alpha}^{P} &= \mu^4\Phi_{,\alpha\alpha} + \mu^2\bar{q}\,\Phi_{,\alpha} + \mu^2\bar{p}^2\,\Phi_{,p} - a^2\left(\frac{1+\nu}{1-\nu}\right)2G\underline{\alpha}T \\
a^2\sigma_{\alpha\beta}^{P} &= \bar{p}\,[-\mu^4\Phi_{,\alpha p} + \mu^2\Phi_{,\alpha} - \mu^2\bar{q}\,\Phi_{,p}] \\
a^2\sigma_{\beta\beta}^{P} &= \mu^4\bar{p}^2\,\Phi_{,pp} - \mu^2(\mu^2 p + \bar{p}^2)\,\Phi_{,p} - \mu^2\bar{q}\,\Phi_{,\alpha} - a^2\left(\frac{1+\nu}{1-\nu}\right)2G\underline{\alpha}T \\
a^2\sigma_{\gamma\gamma}^{P} &= -\mu^2\bar{q}\,\Phi_{,\alpha} + \mu^2(1-qp)\,\Phi_{,p} - a^2\left(\frac{1+\nu}{1-\nu}\right)2G\underline{\alpha}T
\end{aligned}
\tag{22}
$$

In anticipation of establishing stress free boundary conditions by making use of the linear independence of Legendre polynomials and their first derivations the boundary stresses $\sigma_{\alpha\alpha}^{P}$ and $\sigma_{\alpha\beta}^{P}$ are rewritten as

$$
\begin{aligned}
\sigma_{\alpha\alpha}^{P} &= \mu^{-1}\sum_{0}^{\infty} f_n^{P}(\alpha)\,P_n(p) \\
\sigma_{\alpha\beta}^{P} &= \bar{p}\mu^{-1}\sum_{n=1}^{\infty} g_n^{P}(\alpha)P_n'(p)
\end{aligned}
\tag{23}
$$

where $P_n'(p)$ is the first derivative of $P_n(p)$.

In arriving at this form it is necessary to make repeated use of the recurrence relations for the Legendre polynomials as well as equation (16). The $f_n^P(\alpha)$ and $g_n^P(\alpha)$ are given by

$$
\begin{aligned}
f_0^P(\alpha) &= \bar{q}\left(q^2+\frac{1}{6}\right)\ \Omega_0(\alpha) + q\bar{q}\ \bar{\Omega}_0(\alpha) + F_0(\alpha)\\
f_1^P(\alpha) &= -q\bar{q}\ \Omega_0(\alpha) - \bar{q}^2\ \bar{\Omega}_0(\alpha) + F_1(\alpha)\\
f_2^P(\alpha) &= -\frac{1}{6}\bar{q}\ \Omega_0(\alpha) + F_2(\alpha)\\
f_n^P(\alpha) &= F_n(\alpha) \qquad (n \geq 3)
\end{aligned}
\tag{24}
$$

and

$$
\begin{aligned}
g_1^P(\alpha) &= \frac{1}{4}(q^2+1)\ \Omega_0(\alpha) + \frac{1}{4}q\bar{q}\ \bar{\Omega}_0(\alpha) + G_1(\alpha)\\
g_2^P(\alpha) &= \frac{1}{6}q\ \Omega_0(\alpha) - \frac{1}{12}\bar{q}\ \bar{\Omega}_0(\alpha) + G_2(\alpha)\\
g_n^P(\alpha) &= G_n(\alpha) \qquad (n \geq 3)
\end{aligned}
\tag{25}
$$

where

$$
\begin{aligned}
F_n(\alpha) = {} & \frac{n(n-1)(n-2)}{4(2n-1)}\chi_{n-3}(\alpha) - \frac{n(n-1)(2n+5)}{4(2n-1)}q\chi_{n-2}(\alpha)\\
& + \frac{n}{2n-1}\left[\frac{6n^3+5n^2+22n+41}{4(2n+3)} - (n-1)(n-3)q^2\right]\chi_{n-1}(\alpha)\\
& + \left[(n^2+n+1)q^2 - \frac{4n^4+8n^3+25n^2+21n-21}{2(2n-1)(2n+3)}\right]q\chi_n(\alpha)\\
& + \frac{n+1}{2n+3}\left[\frac{6n^3+13n^2+30n-18}{4(2n-1)} - (n+2)(n+4)q^2\right]\chi_{n+1}(\alpha)\\
& - \frac{(n+1)(n+2)(2n-3)}{4(2n+3)}q\chi_{n+2}(\alpha) + \frac{(n+1)(n+2)(n+3)}{4(2n+3)}\chi_{n+3}\\
& - \frac{n(n-1)}{2n-1}\bar{q}\ \bar{\chi}_{n-2}(\alpha) + (2n+1)\left[q^2 - \frac{2n^2+2n-1}{(2n-1)(2n+3)}\right]\bar{q}\ \bar{\chi}_n(\alpha)\\
& - \frac{(n+1)(n+2)}{2n+3}\bar{q}\ \bar{\chi}_{n+2}(\alpha)
\end{aligned}
\tag{26}
$$

$$G_n(\alpha) = \frac{n-1}{4(2n-1)}\,\bar{q}\,\chi_{n-2}(\alpha) + \frac{8n-9}{4(2n-1)}\,q\bar{q}\,\chi_{n-1}(\alpha)$$

$$- \left[\frac{3}{2}q^2 + \frac{4n^2+4n-5}{4(2n-1)(2n+3)}\right]\bar{q}\,\chi_n(\alpha)$$

$$+ \frac{8n+17}{4(2n+3)}\,q\bar{q}\,\chi_{n+1}(\alpha) - \frac{n+2}{4(2n+3)}\,\bar{q}\,\chi_{n+2}(\alpha)$$

$$- \frac{(n-1)(n-2)}{4(2n-1)}\,\bar{\chi}_{n-3}(\alpha) + \frac{n(n-1)}{2(2n-1)}\,q\,\bar{\chi}_{n-2}(\alpha) + \frac{1}{4}\left[(2n-3)q^2\right. \tag{27}$$

$$\left. - \frac{3(n^2+n-1)}{2n+3}\right]\bar{\chi}_{n-1}(\alpha) - \frac{1}{2}(2n+1)\left[q^2 - \frac{2n^2+2n-1}{(2n-1)(2n+3)}\right]q\,\bar{\chi}_n(\alpha)$$

$$+ \frac{1}{4}\left[(2n+5)\,q^2 - \frac{3(n^2+n-1)}{2n-1}\right]\bar{\chi}_{n+1}(\alpha) + \frac{(n+1)(n+2)}{2(2n+3)}\,q\,\chi_{n+2}(\alpha)$$

$$- \frac{(n+2)(n+3)}{4(2n+3)}\,\bar{\chi}_{n+3}(\alpha)$$

with $\chi_n(\alpha)$ and $\Omega_0(\alpha)$ as defined in equation (20) and

$$\bar{\chi}_n(\alpha) = K_n^0 S_n(\alpha) + K_n^1 C_n(\alpha)$$

$$\bar{\Omega}_0(\alpha) = L_n^0 S_n(\alpha) + L_n^1 C_n(\alpha) \tag{28}$$

The above stresses are self equilibrating in that the resultant force on any spherical surface α = constant vanishes.

IV. THE COMPLIMENTARY SOLUTION

Since the particular solution in general will not satisfy the condition of stress free boundaries as required by equation (9) a general or complimentary solution to the homogeneous form of equations (2) and (3) must be obtained. A solution to the homogeneous equation (2) has been obtained by Boussinesq [7] and Papkovich [8] in terms of two harmonic functions one a scalar function and the other a vector function. Since the individual components of a harmonic vector are themselves harmonic functions only in the rectangular Cartesian coordinate system, this is equivalent to formulating the displacement field in Cartesian components in terms of four harmonic functions, V_i and ϕ. The solution is written as

$$2G\, u_i = x_k\, V_{k,i} - (3-4\nu)\, V_i + \phi_{,i} \tag{29}$$

The conditions under which one or two of these functions can be equated to zero have been presented in [9] and [10]. For the axisymmetric torsion free problems under development here only two of the four functions are required. However, since there are several ways to select the pair of functions, all four will be carried in the analysis at this time.

By means of the strain displacement equation (3) and the homogeneous stress-strain equation (4) the Cartesian components of stress can be expressed as

$$\sigma_{ij} = x_k V_{k,ij} - (1-2\nu)\,(V_{i,j} + V_{j,i}) - 2(1-2\nu)\,\delta_{ij}\, V_{k,k} + \phi_{,ij} \tag{30}$$

The procedure for transforming the stresses in equation (3) into the bispherical coordinate system is well defined but lengthy. By treating the components of the harmonic vector V_i as individual functions during the transformation, they remain harmonic functions after the transformation. In the six equations (33) through (38) the functions V_i, $i = 1, 2, 3$, have been replaced by the functions X, Y and Z, respectively. In anticipation of the form of bispherical harmonics, the equations have been modified by the relations

$$\phi_{,\beta} = -\overline{p}\, \phi_{,p} \tag{31}$$

and

$$\phi,_{\beta\beta} = \bar{p}^2\phi,_{pp} - p\phi,_p \tag{32}$$

$$a^2\sigma_{\alpha\alpha} =$$

$$+ a\bar{p}(q-p)\cos\gamma X,_{\alpha\alpha} + (3-2\nu)a\bar{q}\,\bar{p}\cos\gamma X,_\alpha$$

$$- a[2\nu(1-qp)-\bar{p}^2]\bar{p}\cos\gamma X,_p$$

$$+ \frac{2a\nu(q-p)}{\bar{p}}\sin\gamma X,_\gamma + a\bar{p}(q-p)\sin\gamma Y,_{\alpha\alpha}$$

$$+ (3-2\nu)a\bar{q}\,\bar{p}\sin\gamma Y,_\alpha - a\bar{p}[2\nu(1-qp)-\bar{p}^2]\sin\gamma Y,_p \tag{33}$$

$$- 2a\nu\frac{(q-p)}{\bar{p}}\cos\gamma Y,_\gamma - a\bar{q}(q-p)Z,_{\alpha\alpha}$$

$$- a[\bar{q}^2 - 2(1-\nu)(1-qp)]Z,_\alpha - (1-2\nu)a\bar{q}\,\bar{p}^2 Z,_p$$

$$+ (q-p)^2\phi,_{\alpha\alpha} + \bar{q}(q-p)\phi,_\alpha + \bar{p}^2(q-p)\phi,_p$$

$$a^2\sigma_{\alpha\beta} =$$

$$-a\bar{p}^2(q-p)\cos\gamma X,_{\alpha p} + a[\bar{p}^2 + (1-2\nu)(1-qp)]\cos\gamma X,_\alpha$$

$$- 2(1-\nu)a\bar{q}\,\bar{p}^2\cos\gamma X,_p - a\bar{p}^2(q-p)\sin\gamma Y,_{\alpha p}$$

$$+ a[\bar{p}^2+(1-2\nu)(1-qp)]\sin\gamma Y,_\alpha \tag{34}$$

$$- 2(1-\nu)a\bar{q}\,\bar{p}^2\sin\gamma Y,_p + a\bar{q}\,\bar{p}(q-p)Z,_{\alpha p}$$

$$- 2(1-\nu)a\bar{q}\,\bar{p}Z,_\alpha - a\bar{p}[(1-2\nu)(1-qp)-\bar{q}^2]Z,_p$$

$$- \bar{p}(q-p)^2\phi,_{\alpha p} + \bar{p}(q-p)\phi,_\alpha - \bar{q}\,\bar{p}(q-p)\phi,_p$$

$$a^2\,\sigma_{\alpha\gamma} =$$

$$+ a(q-p)\cos\gamma X,_{\alpha\gamma} + (1-2\nu)\,a(q-p)\sin\gamma X,_{\alpha}$$

$$+ 2(1-\nu)a\bar{q}\cos\gamma X,_{\gamma} + a(q-p)\sin\gamma Y,_{\alpha\gamma}$$

$$- (1-2\nu)\,a(q-p)\cos\gamma Y,_{\alpha} + 2(1-\nu)a\bar{q}\sin\gamma Y,_{\gamma} \qquad (35)$$

$$- a\frac{\bar{q}}{\bar{p}}(q-p)Z,_{\alpha\gamma} + \frac{a}{\bar{p}}[(1-2\nu)(1-qp)-\bar{q}^2]Z,_{\gamma}$$

$$+ \frac{(q-p)^2}{\bar{p}}\phi,_{\alpha\gamma} + \frac{\bar{q}}{\bar{p}}(q-p)\phi,_{\gamma}$$

$$a^2\,\sigma_{\beta\beta} =$$

$$+ a\bar{p}^3(q-p)\cos\gamma X,_{pp} - (1-2\nu)a\bar{q}\,\bar{p}\cos\gamma X,_{\alpha}$$

$$- a\bar{p}[2\bar{p}^2 + (1-2\nu)(1-qp)]\cos\gamma X,_{p}$$

$$+ 2\nu a\frac{(q-p)}{\bar{p}}\sin\gamma X,_{\gamma} + a\bar{p}^3(q-p)\sin\gamma Y,_{pp}$$

$$- (1-2\nu)a\bar{q}\,\bar{p}\sin\gamma Y,_{\alpha} - a\bar{p}[2\bar{p}^2 + (1-2\nu)(1-qp)]\sin\gamma Y,_{p} \qquad (36)$$

$$- 2\nu a\frac{(q-p)}{\bar{p}}\cos\gamma Y,_{\gamma} - a\bar{q}\,\bar{p}^2(q-p)Z,_{pp}$$

$$+ a[\bar{q}^2 + 2\nu(1-qp)]Z,_{\alpha} + a\bar{q}[(q-p)p + (3-2\nu)\bar{p}^2]Z,_{p}$$

$$+ (q-p)^2\bar{p}^2\phi,_{pp} - \bar{q}(q-p)\phi,_{\alpha} - (q-p)(1+qp-2p^2)\phi,_{p}$$

$$a^2\,\sigma_{\beta\gamma} =$$

$$- a\bar{p}(q-p)\cos\gamma X,_{p\gamma} - (1-2\nu)\,a\bar{p}(q-p)\sin\gamma X,_{p}$$

$$+ 2(1-\nu)\,a\frac{(1-qp)}{\bar{p}}\cos\gamma X,_{\gamma} - a\bar{p}(q-p)\sin\gamma Y,_{p\gamma} \qquad (37)$$

$$+ (1-2\nu)a\bar{p}(q-p)\cos\gamma Y,_p + 2(1-\nu)a\frac{(1-qp)}{\bar{p}}\sin\gamma Y,_\gamma$$

$$+ a\bar{q}(q-p)Z,_{p\gamma} - a\frac{\bar{q}}{\bar{p}^2}[(1-qp) + (1-2\nu)\bar{p}^2]Z,_\gamma \qquad (37)$$

$$- (q-p)^2\phi,_{p\gamma} + \frac{(q-p)(1-qp)}{\bar{p}^2}\phi,_\gamma$$

$$a^2\sigma_{\gamma\gamma} =$$

$$+ a\frac{(q-p)}{\bar{p}}\cos\gamma X,_{\gamma\gamma} - (1-2\nu)a\bar{q}\,\bar{p}\cos\gamma X,_\alpha$$

$$+ a\bar{p}(1-2\nu)(1-qp)\cos\gamma X,_p + 2(1-\nu)a\frac{(q-p)}{\bar{p}}\sin\gamma X,_\gamma$$

$$+ a\frac{(q-p)}{\bar{p}}\sin\gamma Y,_{\gamma\gamma} - (1-2\nu)a\bar{q}\,\bar{p}\sin\gamma Y,_\alpha \qquad (38)$$

$$+ a\bar{p}(1-2\nu)(1-qp)\sin\gamma Y,_p - 2(1-\nu)a\frac{(q-p)}{\bar{p}}\cos\gamma Y,_\gamma$$

$$- a(q-p)\frac{\bar{q}}{\bar{p}^2}Z,_{\gamma\gamma} + a[\bar{q}^2 + 2\nu(1-qp)]Z,_\alpha$$

$$+ a\bar{q}[2\nu\bar{p}^2 + qp - 1]Z,_p + \frac{(q-p)^2}{\bar{p}^2}\phi,_{\gamma\gamma}$$

$$- \bar{q}(q-p)\phi,_\alpha + (q-p)(1-qp)\phi,_p$$

As pointed out earlier, for axial symmetry the stresses $\sigma_{\alpha\alpha}$, $\sigma_{\alpha\beta}$, $\sigma_{\beta\beta}$, and $\sigma_{\gamma\gamma}$ must be independent of γ and the stresses $\sigma_{\alpha\gamma}$ and $\sigma_{\beta\gamma}$ must be zero. In [2] and [3] this was accomplished by equating the functions X and Y to zero and using axisymmetric potential functions of the form given in equation (10). If the functions ϕ and ψ are given by

$$\phi = \mu\sum_0^\infty [D_n^0 C_n(\alpha) + D_n^1 S_n(\alpha)]P_n(p) = \mu\sum_0^\infty D_n P_n(p)$$

$$\psi = \mu\sum_0^\infty [E_n^0 C_n(\alpha) + E_n^1 S_n(\alpha)]P_n(p) = \mu\sum_0^\infty E_n P_n(p) \qquad (39)$$

then the stresses will be of the form

$$\sigma^c = \sum_{n=0}^{\infty} \bar{\sigma}_n^c \tag{40}$$

where the $\bar{\sigma}_n^c$ are

$$\begin{aligned}\bar{\sigma}^c_{\alpha\alpha n} = \frac{1}{a\mu}\Bigg\{&\frac{1}{4}\big[(k^2-4+8\nu)\mu^2 q\bar{q} - (k^2+2-4\nu)\mu^2\bar{q}p \\ &+ (7-8\nu)\bar{q}^3\big]E_nP_n(p) + \mu^2 k\big[\bar{q}^2-(1-\nu)(1-qp)\big]\bar{E}_nP_n(p) \\ &+ (1-2\nu)\bar{q}\,\bar{p}^2\mu^2 E_nP_n'(p)\Big\} + \frac{\mu}{a^2}\Bigg\{\frac{1}{4}\big[(k^2+1)\mu^4 \\ &+ 2\bar{q}^2-\bar{p}^2\big]D_nP_n(p) + k\bar{q}\mu^2\bar{D}_nP_n(p) \\ &+ \bar{p}^2\mu^2 D_nP_n(p)\Bigg\}\end{aligned} \tag{41}$$

$$\begin{aligned}\bar{\sigma}_{\beta\beta n} = \frac{1}{a\mu}\Bigg\{&\frac{1}{4}\big[(k^2-6+8\nu)\mu^2 q\bar{q} - (k^2+6-4\nu)\mu^2\bar{q}p \\ &+ (7-8\nu)\bar{q}^3\big]E_nP_n(p) + \big[(3-2\nu)\bar{p}^2+1-qp\big]\mu^2\bar{q}\,E_nP_n'(p) \\ &+ \frac{k}{2}\big[\bar{q}^2+2\nu(1-qp)\big]\bar{E}_nP_n(p)\Big\} + \frac{\mu^2}{a^2}\Bigg\{-\frac{1}{4}\big[k^2\mu^4+\bar{q}^2 \\ &- 2\bar{p}^2\big]D_nP_n(p) + \mu^2(\mu^2 p-2\bar{p}^2)D_nP_n'(p) \\ &- \frac{k}{2}\mu\bar{q}\,\bar{D}_nP_n(p)\Bigg\}\end{aligned} \tag{42}$$

$$\begin{aligned}\bar{\sigma}^c_{\gamma\gamma n} = \frac{\mu}{a}\Bigg\{&\frac{1}{2}(q-2\nu p)E_nP_n(p) + (qp-1+2\nu\bar{p}^2)\bar{q}\,E_nP_n'(p) \\ &+ \frac{k}{2}\big[\bar{q}^2+2\nu(1-qp)\big]\bar{E}_nP_n(p)\Big\} - \frac{\mu^3}{a^2}\Bigg\{\frac{1}{2}q\,D_nP_n(p) \\ &+ \frac{1}{2}k\bar{q}\,\bar{D}_nP_n(p) - (1-qp)D_nP_n'(p)\Bigg\}\end{aligned} \tag{43}$$

$$\bar{\sigma}^{c}_{\alpha\beta n} = \frac{\bar{p}}{a\mu}\left\{\frac{1}{4}\left[2(1-2\nu)\mu^2 q-(7-8\nu)\bar{q}^2\right]E_n P_n(p)\right.$$

$$+\frac{k}{2}\mu^4\bar{q}\,\bar{E}_n P'_n(p)-\frac{k}{4}(5-4\nu)\mu^2\bar{q}\,\bar{E}_n P_n(p)$$

$$\left.+\frac{1}{2}\left[3\bar{q}^2-2(1-2\nu)(1-qp)\right]\mu^2 E_n P'_n(p)\right\} \qquad (44)$$

$$+\frac{\mu\bar{p}}{4a^2}\left\{3(\bar{q}D_n+k\mu^2\bar{D}_n)P_n(p)\right.$$

$$\left.-2\mu^2(3\bar{q}D_n+k\mu^2\bar{D}_n)P'_n(p)\right\}$$

Where D_n and E_n are as defined in equation (39) and

$$\bar{D}_n = D^0_n S_n(a) + D^1_n C_n(a)$$

$$\bar{E}_n = E^0_n S_n(a) + E^1_n C_n(a) \qquad (45)$$

In order to apply the boundary conditions given in equation (9), however, the stresses in equations (41) and (44) must be written in the same form as the corresponding stresses in the particular solution as given in equation (23). This requires the same lengthy procedure as used for the particular solution. Denoting the stresses as

$$\sigma^{c}_{\alpha a} = \frac{1}{\mu}\sum_{0}^{\infty} f^{c}_n(a)\,P_n(p)$$

$$\sigma^{c}_{\alpha\beta} = \frac{\bar{p}}{\mu}\sum_{0}^{\infty} g^{c}_n(a)\,P'_n(p) \qquad (46)$$

the functions $f^c_n(a)$ and $g^c_n(a)$ are found to be (these equations are as corrected in version of ones developed in [2])

$$f^{c}_n(a) = -\frac{(k-1)(k-3)(k-5)}{32a^2(k-2)}D_{n-3}+\frac{(k-1)(k-3)}{16a^2(k-2)}\left[(3k-8)qD_{n-2}+4\bar{q}\,\bar{D}_{n-2}\right]$$

$$-\frac{(k-1)(k-3)}{16a(k-2)}\left[(k-2-4\nu)\bar{q}E_{n-2}-4(1-\nu)q\,\bar{E}_{n-2}\right] \qquad (47)$$

$$+\frac{1}{a^2}\left\{-\frac{(k-1)}{32(k^2-4)}\left[3k^3-4k^2-9k+18\right.\right.$$

$$\left.\left.-4(k+2)[(k-2)(3k-4)q^2+3\bar{q}^2]\right]D_{n-1}-(k-1)q\bar{q}\bar{D}_{n-1}\right\}$$

$$+\frac{(k-1)}{4a}\left\{\frac{(k-2)^2+(k-4)(1-2\nu)}{k-2}\,q\bar{q}E_{n-1}\right.$$

$$\left.+[2\bar{q}^2-2(1-\nu)(1+q^2)]\bar{E}_{n-1}\right\}+\frac{1}{8a^2}\left\{\left[2(k^2q^2+3\bar{q}^2)q\right.\right.$$

$$\left.\left.+\frac{(3k^4-9k^2-8)}{(k^2-4)}q\right]D_n+4k\bar{q}\left[2q^2+\frac{k^2-3}{k^2-4}\right]\bar{D}_n\right\}$$

$$-\frac{1}{8a}\left\{\bar{q}\left[2(k^2-4+8\nu)q^2+\frac{k^2(k^2-3)-4(1-2\nu)}{(k^2-4)}\right.\right.$$

$$\left.\left.+2(7-8\nu)\bar{q}^2\right]E_n+4kq\left[2(\bar{q}^2-1+\nu)-(1-\nu)\frac{k^2-3}{k^2-4}\right]\bar{E}_n\right. \qquad (47)$$

$$+\frac{1}{a^2}\left\{-\frac{(k+1)}{32(k^2-4)}\left[3k^3+4k^2-9k-18\right.\right.$$

$$\left.\left.-4(k-2)[(k+2)(3k+4)q^2+3\bar{q}^2]\right]D_{n+1}-(k+1)q\bar{q}\bar{D}_{n+1}\right\}$$

$$+\frac{(k+1)}{4a}\left\{\frac{(k+2)^2-(k+4)(1-2\nu)}{(k+2)}\,q\bar{q}E_{n+1}\right.$$

$$\left.+[2\bar{q}^2-2(1-\nu)(1+q^2)]\bar{E}_{n+1}\right\}$$

$$+\frac{(k+1)(k+3)}{16a^2(k+2)}[(3k+8)qD_{n+2}+4\bar{q}\bar{D}_{n+2}]$$

$$-\frac{(k+1)(k+3)(k+5)}{32a^2(k+2)}D_{n+3}-\frac{(k+1)(k+2)}{16a(k+2)}[(k+2+4\nu)\bar{q}E_{n+2}$$

$$-4(1-\nu)q\bar{E}_{n+2}] \qquad , \; n \geq 0$$

$$
\begin{aligned}
g_n^c(a) = {} & \frac{(k-3)(k-5)}{16(k-2)a^2}\,\overline{D}_{n-3} - \frac{3(k-3)}{8a^2(k-2)}\,[\overline{q}\,D_{n-2} + (k-3)q\,\overline{D}_{n-2}] \\
& + \frac{(k-3)}{8a\,(k-2)}\,[(k-4\nu)\,\overline{q}\,\overline{E}_{n-2} - 2(1-2\nu)q\,E_{n-2}] \\
& + \frac{1}{a^2}\left\{\frac{3(2k-5)}{4\,(k-2)}\,q\,\overline{q}\,D_{n-1} + \frac{3}{16}\left[4(k-2)q^2\right.\right. \\
& \left.\left. + \frac{(k^2-5)}{(k+2)}\right]\overline{D}_{n-1}\right\} + \frac{1}{4a}\left\{2\,\frac{(1-2\nu)}{(k-2)}\,[(k-4)q^2+k-1\,]E_{n-1}\right. \\
& \left. - 3\,\overline{q}^{\,2}E_{n-1} - (2k-1-4\nu)q\,\overline{q}\,\overline{E}_{n-1}\right\} \\
& - \frac{1}{4a^2}\left\{3\overline{q}\left[\frac{k^2-6}{k^2-4} + 2q^2\right]D_n + kq\left[3\,\frac{k^2-5}{k^2-4} + q^2\right]\overline{D}_n\right\} \\
& + \frac{1}{4a}\left\{2q\left[3\,\overline{q}^{\,2} - (1-2\nu)\,\frac{(3k^2-14)}{(k^2-4)}\right]E_n\right. \\
& \left. + \frac{k}{k^2-4}\,[2(1-2\nu) + (k^2-4)(1+2q^2)\,]\overline{q}\,\overline{E}_n\right\} \\
& + \frac{1}{a^2}\left\{\frac{3(2k+5)}{4(k+2)}\,q\,\overline{q}\,D_{n+1} + \frac{3}{16}\left[4(k+2)q^2\right.\right. \\
& \left.\left. + \frac{k^2-5}{k-2}\right]\overline{D}_{n+1}\right\} + \frac{1}{4a}\left\{2\,\frac{(1-2\nu)}{(k-2)}\,[(k+4)q^2\right. \\
& \left. + k+1\,]E_{n+1} - 3\overline{q}^{\,2}E_{n+1} - (2k+1+4\nu)q\,\overline{q}\,\overline{E}_{n+1}\right\} \\
& - \frac{3(k+3)}{8a^2(k+2)}\,[\overline{q}\,D_{n+2} + (k+3)q\,\overline{D}_{n+2}] \\
& + \frac{(k+3)}{8a(k+2)}\,[(k+4\nu)\,\overline{q}\,\overline{E}_{n+2} - 2(1-2\nu)q\,E_{n+2}] \\
& + \frac{(k+3)(k+5)}{16a^2(k+2)}\,\overline{D}_{n+3} \qquad , \; n \geq 1
\end{aligned}
\tag{48}
$$

From equations (23) and (46) it is seen that the boundary equation (9) can be expressed as

$$f_n^c(0) + f_n^p(0) = 0$$

$$f_n^c(a_c) + f_n^p(a_c) = 0$$

$$g_n^c(0) + g_n^p(0) = 0$$

$$g_n^c(a_c) + g_n^p(a_c) = 0$$

Once the temperature distribution is known, the terms $f_n^p(0)$, $f_n^p(a_c)$, $g_n^p(0)$, and $g_n^p(a_c)$ can be evaluated from equations (24), (25), (26), and (27). Consequently, equation (49) is an infinite set of linear algebraic equations in which the four types of constants D_n^0, D_n^1, E_n^0, and E_n^1 are the unknowns. Unfortunately, the convergence of the solution of this set is rather slow so that in a practical sense it is very difficult to obtain meaningful numerical results from it.

It was at this point that Dr. Warren succeeded in applying the redundant solution method to the particular solution and it was decided to attempt to apply it to the complementary solution.

V. APPLICATION OF REDUNDANT SOLUTION METHOD TO THE COMPLEMENTARY SOLUTION

The basic idea of the redundant solution method was demonstrated with equation (21); namely to find a set of solutions, some of which are redundant which can be truncated to yield homogeneous equations to correspond to the truncation of the series coefficients of the right hand side. Studies of the temperature series revealed that adequate description of the temperature field was achieved by using only the constants T_0^1, T_1^1, and T_2^1; in other words truncating the series at n=2. An examination of equations (24), (25), (26) and (27) shows that if the temperature series were to be truncated at n=2, the series for the particular solution of the stresses would be truncated at n=4.

With $f^P{}_n(\alpha)$ and $g^P{}_n(\alpha)$ truncated at n=4 it follows from equation (49) that there would be only eighteen equations which were not homogeneous. Equations (47) and (48) show that the ten constants

$$D_0^0,\ D_0^1,\ D_1^0,\ D_1^1$$

$$E_0^0,\ E_0^1,\ E_1^0,\ E_1^1,\ E_2^0,\ E_2^1$$

are contained only in the expressions for $f^C{}_n(\alpha)$ and $g^C{}_n(\alpha)$ for $n \leq 4$. Consequently, if it were possible to find eight more independent solutions whose constants were not involved in $f^C{}_n(\alpha)$ and $g^C{}_n(\alpha)$ for $n \geq 5$, then the redundant solution method could be applied to the complementary solution.

At the beginning there was some doubt that this method would work. The complementary solution is quite different from the particular solution where any function is sought which will render the equation homogeneous. Then, too, there was the matter of the uniqueness therem of the classical theory of linear elasticity which with the orthogonal, linearly independent Legendre functions meant that the coefficients in the Fourier-Legendre series had to be unique. However, in view of the rather large number of constants involved in the coefficient of each of the Legendre functions and the presence of an infinite set of equations, it was not at all certain that the method of redundant solutions would not work. After weighing these factors with the benefits to be gained if the method were successful, it was decided to try it.

The success of the method depended not only on being able to find eight more solutions whose constants were not involved in $f^C{}_n(\alpha)$ and $g^C{}_n(\alpha)$ for $n \geq 5$ but also all eight additional solutions had to be linearly

independent of each other and independent of the ten suitable terms taken from the previously obtained solution. Certain solutions such as the Galerkin vector and the Maxwell-Morra solution were not tried for example because they are known to be related to the Boussinesq-Papkovich solution.

One source which was selected was an axially symmetric stress function apparently introduced by Love [11], in which the stresses in cylindrical coordinates are given by

$$\begin{aligned}
\sigma_{rr} &= \frac{\partial}{\partial z}\left[\nu\nabla^2\psi - \frac{\partial^2\psi}{\partial r^2}\right] \\
\sigma_{\theta\theta} &= \frac{\partial}{\partial z}\left[\nu\nabla^2\psi - \frac{1}{r}\frac{\partial\psi}{\partial r}\right] \\
\sigma_{zz} &= \frac{\partial}{\partial z}\left[(2-\nu)\nabla^2\psi - \frac{\partial^2\psi}{\partial z^2}\right] \\
\sigma_{rz} &= \frac{\partial}{\partial r}\left[(1-\nu)\nabla^2\psi - \frac{\partial^2\psi}{\partial z^2}\right]
\end{aligned} \tag{50}$$

Where the stress function ψ satisfies the biharmonic equation

$$\nabla^4\psi = 0 \tag{51}$$

From previous discussion it is evident that the function ψ will be biharmonic if

$$\psi = r^2\psi_1 + z\,\psi_2 + \psi_3 \tag{52}$$

where ψ_1, ψ_2, and ψ_3 are all axisymmetric harmonic functions. After transforming the stresses given by equation (50) into the bispherical coordinate system it was found that the following function satisfied the first requirement in that the constants were not involved in any equation for $n \geq 5$.

$$\begin{aligned}
\psi_1 &= \mu\{[A_0C_0(\alpha) + B_0S_0(\alpha)]P_0(p) + [A_1C_1(\alpha) + B_1S_1(\alpha)]P_1(p)\} \\
\psi_2 &= \mu\{[C_0C_0(\alpha) + D_0S_0(\alpha)]P_0(p) + [C_1C_1(\alpha) + D_1S_1(\alpha)]P_1(p)\} \\
\psi_3 &= \mu\{[E_0C_0(\alpha) + F_0S_0(\alpha)P_0(p)\}
\end{aligned} \tag{53}$$

where A_0, B_0, A_1, B_1, C_0, D_0, C_1, D_1, E_0, and F_0 are all constants. This corresponds to ten extra solutions and only eight are required but it was suspected that some of these might not be independent. Equations (53)

were substituted into the proper stress equations in the bispherical coordinate system and conditioned with the recurrence formulae for Legendre functions so the stresses had the forms

$$\sigma^{c}_{\alpha\alpha} = \frac{1}{\mu} \sum_{0}^{4} f^{c}_{n}(\alpha) P_{n}(p)$$
$$\sigma^{c}_{\alpha\beta} = \frac{\bar{p}}{\mu} \sum_{1}^{4} g^{c}_{n}(\alpha) P^{1}_{n}(p) \qquad (54)$$

From the general form of the bispherical potential function,

$$\psi = \mu \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} [A_{mn}\cosh(n+\tfrac{1}{2})\alpha + B_{mn}\sinh(n+\tfrac{1}{2})\alpha]P^{m}_{n}(\cos\beta)\cos m\gamma \qquad (55)$$

it was found that another set of axisymmetric solutions could be constructed from the Boussinesq-Papkovich potentials by taking the functions X and Y in equations (33) through (38) to be

$$X = \mu \sum_{0}^{\infty} [\tilde{A}_{n}\cosh(n+\tfrac{1}{2})\alpha + \tilde{B}_{n}\sinh(n+\tfrac{1}{2})\alpha]P^{1}_{n}(p)\cos\gamma$$
$$Y = \mu \sum_{0}^{\infty} [\tilde{A}_{n}\cosh(n+\tfrac{1}{2})\alpha + \tilde{B}_{n}\sinh(n+\tfrac{1}{2})\alpha]P^{1}_{n}(p)\sin\gamma \qquad (56)$$

The resulting equations for the stresses $\sigma_{\alpha\alpha}$, $\sigma_{\alpha\beta}$, $\sigma_{\beta\beta}$, $\sigma_{\gamma\gamma}$ are independent of γ and the stresses $\sigma_{\alpha\gamma}$ and $\sigma_{\beta\gamma}$ are zero. In equation (56) the $P^{1}_{n}(p)$ are the associated Legendre functions of order one and are related to the Legendre functions of order zero by the relation, see e.g. [6] p. 323,

$$P^{1}_{n}(p) = \bar{p}\frac{d}{dp}(P_{n}(p)) = \bar{p}P'_{n}(p) \qquad (57)$$

These functions complicate the development of the equations for the stresses considerably and after these equations were developed it was found that the terms which satisfied equations (54) were those corresponding to $\tilde{A}_1$ and $\tilde{B}_1$. Note that $\tilde{A}_0$ and $\tilde{B}_0$ are of no value since $P^{1}_{0}(p)$ is zero.

At this point twelve additional solutions had been found which satisfied equation (54). This made an aggregate of twenty-two solutions from which it was necessary to find a set of eighteen which were linearly independent.

From the development of these solutions it can be shown that the twenty-two solutions are actually made up of eleven pairs of solutions which are linearly independent of each other. Thus the task was one of finding nine linearly independent pairs from a set of eleven pairs. To do this, a matrix of the solution was first prepared in which each row corresponded to the appropriate equation from equation (49). The value of a_c used was 2.0 and the order of the rows was $f_0^c(0)$, $f_0^c(2)$, $g_1^c(0)$, $g_1^c(2)$, $f_1^c(0)$, $f_1^c(2)$, $g_2^c(0)$, $g_2^c(2)$, $f_2^c(0)$, $f_2^c(2)$, $g_3^c(0)$, $g_3^c(2)$, $f_3^c(0)$, $f_3^c(2)$, $g_4^c(0)$, $g_4^c(2)$, $f_4^c(0)$, $f_4^c(2)$. Each column of this twenty-two column, eighteen row matrix contained the numerical coefficients corresponding to one of the twenty-two solutions. The tests for linear independence consisted of selecting eighteen columns from the matrix and forming an eighteen by eighteen determinant which was evaluated. If the value of the determinant was very small compared to typical non-zero elements in the solutions, then the determinant was considered singular indicating that linear dependence existed in the set of solutions selected.

From a set of eleven pairs, it is possible to select combinations of nine pairs fifty-five different ways. The search was started using a Burroughs 205 computer which the University of Denver had at that time. The first results were inconclusive and very time consuming. The 205 required twenty minutes to evaluate each determinant. The equations were being continually reexamined and due to their complex nature small errors were found and corrected.

After this had proceded for awhile the Burroughs B5000 computer became available at the Marathon Oil Company. When the program and data had been converted to be acceptable to this machine it tested all possible fifty-five combinations in less than five minutes. Although the performance was spectacular, the results were disappointing; all of the fifty-five determinants were singular and, therefore, all possible combinations possessed linear dependence and the redundant solution method failed.

It was then hoped that it might be possible to find a set of sixteen solutions which would be linearly independent. This would significantly reduce the complexity of the truncation process and greatly speed convergence. There are one hundred sixty-five ways to select eight pairs of objects from a population of eleven pairs. This is further complicated by the fact that an array consisting of eighteen rows and sixteen columns cannot form a determinant. To overcome this, two unit diagonals, columns consisting of zeros except for ones on the main diagonal, were added to the array. To be completely certain of the check, two determinants were calculated for each set of arrays; one with unit diagonals

added to the left side, the other with unit diagonals added to the right. For the set to be linearly dependent, both determinants had to be zero. Unfortunately, this proved to be the case. Searches for smaller sets of linearly independent solutions were not attempted since they would represent less improvement and it seemed very unlikely that the searches would be successful.

VI. DEVELOPMENTS AFTER TRIAL OF THE REDUNDANT SOLUTION METHOD

After the failure of the redundant solution method, it was decided to complete the problem using the complementary solution from [2]. Development of the program has proved to be a significant task since each phase of the operation has to be verified numerically before the next can be attempted. The program is being written in the extended ALGOL 60 language for the Burroughs B5500 computer. Extensive use is made of PROCEDURES (similar to SUBROUTINES in FORTRAN) so that parts of this program can be used readily in related programs with very little or no modification.

The development of PROCEDURES for the particular solution proceded quite smoothly but the complementary solution has been another matter. The first attempt used equations (47) and (48) to generate the linear algebraic equations from which the constants D_n^0, D_n^1, E_n^0, and E_n^1 were to be calculated. Unfortunately, the convergence was extremely slow and the process of truncation appeared to give answers that differed widely and no basis could be found would specify the method of truncation to be used.

Since this appeared unlikely to yield a solution it was decided to investigate some earlier work of Sternberg and Sadowsky [3]. This paper dealt with two problems of an infinite medium containing two equal sized, stress free cavities. The medium at infinity was subjected to 1) hydrostatic tension or 2) uniaxial tension parallel to the axis of the cavities. This is a considerably simpler problem since it requires only two boundary conditions, the second of equations (9), instead of four. Consequently, only parts of the potential functions of equation (39) were required, namely,

$$\phi = \mu \sum_0^\infty D_n^0 C_n(\alpha) P_n(p) = \mu \sum_0^\infty d_n^0$$

$$\psi = \mu \sum_0^\infty E_n^1 S_n(\alpha) P_n(p) = \mu \sum_0^\infty e_n^1 \qquad (58)$$

Through ingenious transformations given by

$$a_n^0 = \sum_0^n (n+1-i) d_n^0, \qquad b_n^0 = \frac{2}{k^2-1} \sum_0^n (e_n^1 - e_i^1) \qquad (59)$$

so that

$$\phi = \mu \sum_{0}^{\infty} A_n^0 a_n^0 , \qquad \psi = \mu \sum_{1}^{\infty} B_n^1 b_n^1 \tag{60}$$

the number of coefficients contained in each equation was reduced noticeably. Consequently, the band width of non-zero coefficients in the boundary equations is narrower and the process of truncation is less severe.

To test the validity of this solution the work of Sternberg and Sadowsky was programmed on the Burroughs B5500. Only limited numerical results for the case of hydrostatic tension at infinity were presented in the paper. These results were verified and extended to include a great many more geometrical configurations. For this loading it was found that the stress concentration could be made arbitrarily large as the separation distance between the cavities was progressively decreased. Figure 3 illustrates the variation of the stress concentration factor with separation distance.

The case of uniaxied tension at infinity was also studied. Here the stress concentration is nearly independent of separation distance. The maximum stress is a circumferential one and occurs on the cavity at the maximum distance from the axis of symmetry. For practical purposes the value of this stress concentration factor is the same as for a single cavity under the same loading. As the two cavities approach each other the region between them becomes very nearly stress free.

Since the complimentary solution of equation (60) does not involve sufficient constants it had to be modified for application to the thermal stress problem. This turned out to be relatively straight forward since the solution desired must have the form of equation (39). With subsequent transformation as given by equations (59) and (60). Fortunately, it was found to be unnecessary to repeat the tedious transformation for the second set of solutions since some simple relations were found by which the transformed equations of the first set could be modified to give the results for the second set.

It appears that this complementary solution will ultimately satisfy the requirements of the problem. Not all of the problems have as yet been overcome but the truncation difficulty is greatly alleviated. The primary problem is the annihilation of the stresses on the boundary. It is believed that this is due either to a small, as yet undetected,

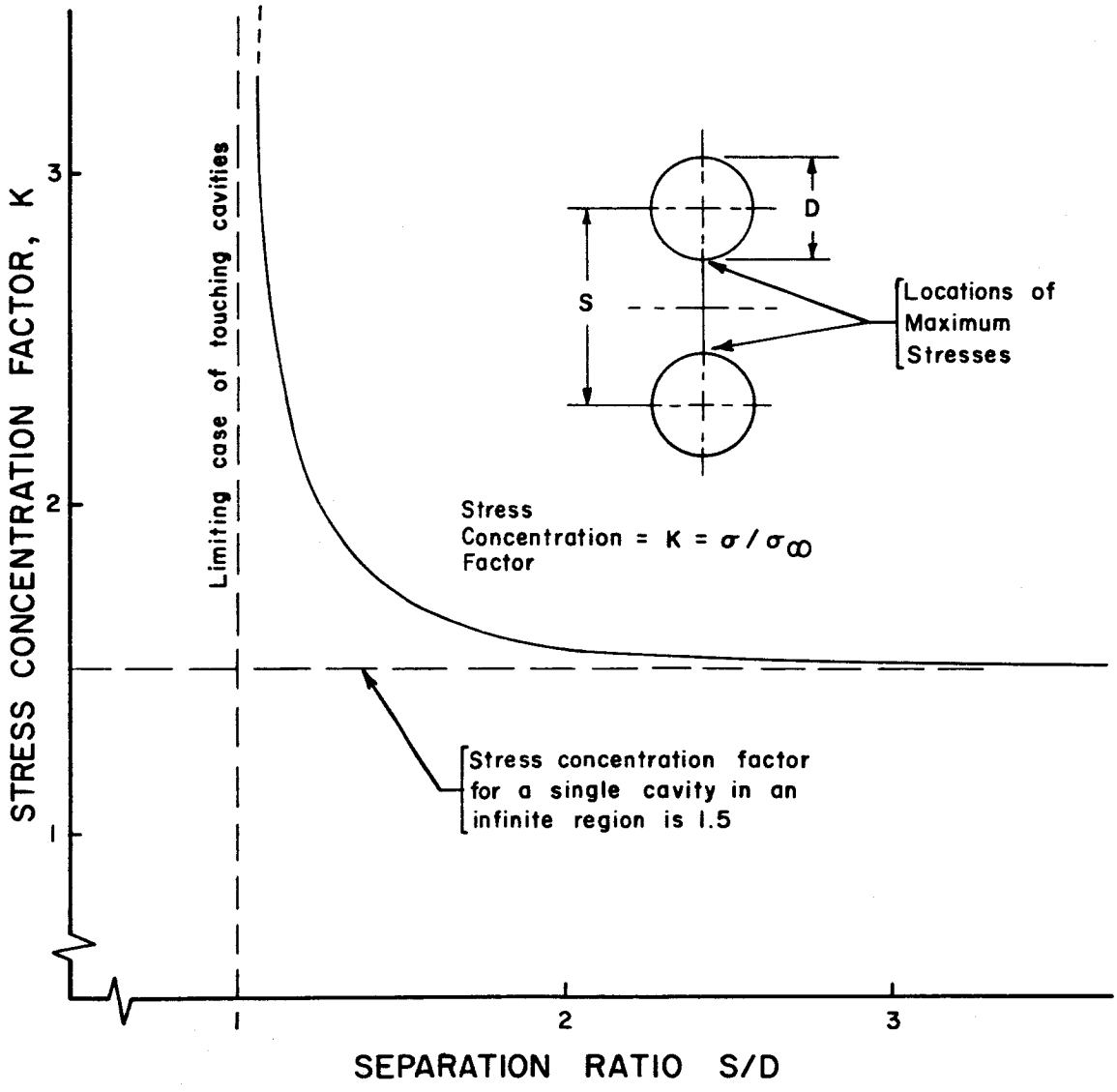


Figure 3. Stress Concentration Factor Vs. Separation Distance for Two Equal Sized Spherical Cavities in an Infinity Medium Under Hydrostatic Loading at Infinity, σ_∞.

programming error or perhaps a need for more double precision operations in the calculation of the stresses.

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FINAL REPORT

DEVELOPMENT OF ADAPTIVE SYSTEM APPLICATION CRITERION

A Research Project Supported by a
NASA Grant in the Space-Related Sciences

NsG-518

Project No. DRI-604

University of Denver
June 1965

SUBMITTED BY:

M. L. Moe
Principal Investigator,
Electronics Division and
Electrical Engineering
Department

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I. INTRODUCTION

This final report gives a summary of the procedures used in the investigation. An annotated bibliography of some of the literature studied during the course of this investigation is given in Section VI.

The investigation required several computer programs which were not previously available. This programming was complicated by a change in computers at the University several months after the investigation began. However, the change from a Burroughs 205 to a Burroughs 5500 had two definite advantages that outweighed the effort of reprogramming. The improved programming language and increased computer speed made it possible to write more flexible programs to aid the investigation. Also all programs were written and checked out during the installation period of the computer when no charges were made for computer time which resulted in a substantial savings for the project. A description of the programs written is given in Section IV.

The principal investigator was aided in this study by Mr. George Koltko, Graduate Research Assistant. Additional results will be presented in a thesis to be submitted by Mr. Koltko as well as a paper to be submitted for publication.

II. OBJECTIVE

The objective of this study was the development of a quantitative design criterion for control systems which can be used to determine when an adaptive system is needed to control a plant with varying parameters. A study of the literature and some preliminary investigations led to the conclusion that the most difficult task is the specification of the best non-adaptive system. Once this best non-adaptive or fixed-compensation system (often termed passive adaptive in the literature) is determined it is evident whether or not all the specifications can be met with a fixed compensator. The possible improvements which any particular adaptive scheme might offer can then be determined by simulation.

III. PROCEDURE

The basic system configuration under study is shown in Figure 1. The plant is assumed to have parameters which vary over some prescribed domain. The usual justification for the use of adaptive control is that it tends to give invariant performance when the plant is varying. See Horowitz[1] for a discussion of examples of such statements. It is very easy to show, however, that parameter variations alone do not provide a valid reason for using an adaptive controller. An example will demonstrate this.

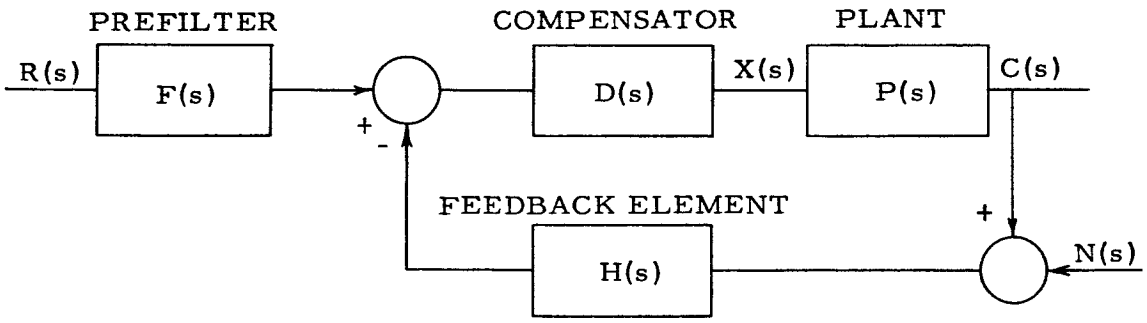

Figure 1. Basic System Configuration

Example 1

Consider a plant which has a transfer function, P(s), given by

$$P(s) = \frac{Kp}{s(1 + \tau s)} \qquad \begin{matrix} 0.5 \leq Kp \leq 5 \\ 0.5 \leq \tau \leq 4 \end{matrix} \tag{1}$$

The region of parameter variation for the plant is shown in Figure 2. Let the desired system behavior be represented by a model which has some prespecified transfer function, M(s). The problem then, is that of finding a compensator which will keep the closed loop system performance suitably close to the performance of the model. One simple technique, which will work for this problem, is to use the model as a prefilter and use a high gain in the loop. This configuration is shown in Figure 3. The compensation, D(s), is simply an amplifier with gain K_1. The closed loop transfer function or transmission function T(s), becomes

$$T(s) = \frac{C(s)}{R(s)} = M(s)\left[\frac{K_1 P(s)}{1 + K_1 P(s)}\right] \tag{2}$$

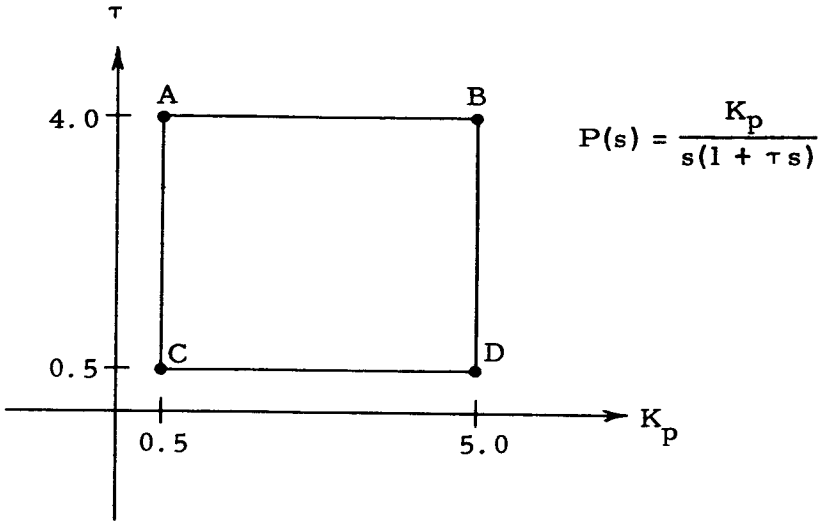

Figure 2. Region of Parameter Variation for Example Plant

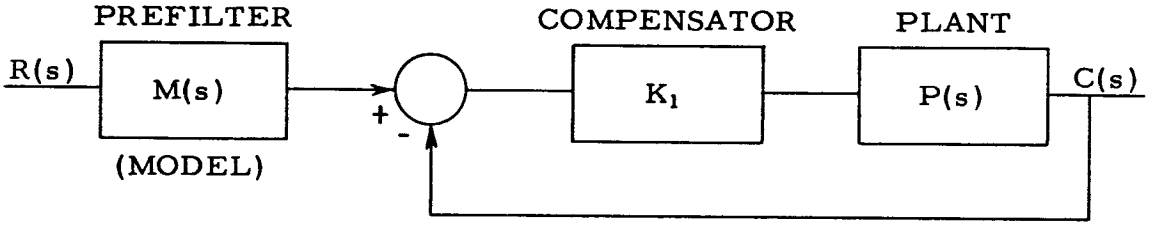

Figure 3. Simple Compensation for the Parameter Variations Shown in Figure 2

As K_1 becomes large the term in brackets becomes close to unity for all frequencies of interest and the transfer function T(s) becomes equal to M(s) for all practical purposes. Thus as K_1 becomes large the effect of the parameter variations becomes negligible and the problem, as stated, is solved. The same techniques will work for higher order systems as long as proper compensation is put into the loop to insure stability. Thus, an adaptive controller cannot be justified for this problem.

The high gain compensation technique, which was used in the above example to demonstrate that parameter variations alone are not sufficient justification for adaptive control, can also give a clue to situations when adaptive control might be needed. There is an obvious problem with the high gain technique as described. In order to keep the output C(s) at the desired value a very large input signal to the plant is required. This means there is likely to be a severe problem with plant saturation. Also, if there is any noise introduced by the transducer used to measure the output signal for the feedback path it is amplified by K_1 and hence could cause large signals which would tend to saturate the plant. This transducer noise, represented by N(s) in Figure 4, is not attenuated by the system since

$$\frac{C(s)}{N(s)} = \frac{-K_1 P(s)}{1 + K_1 P(s)} \tag{3}$$

which is approximately unity for large K_1.

The ability of the high gain compensation system to perform properly is then limited by constraints on the maximum signal magnitude allowed as an input to the plant and any requirements on the filtering of transducer noise.

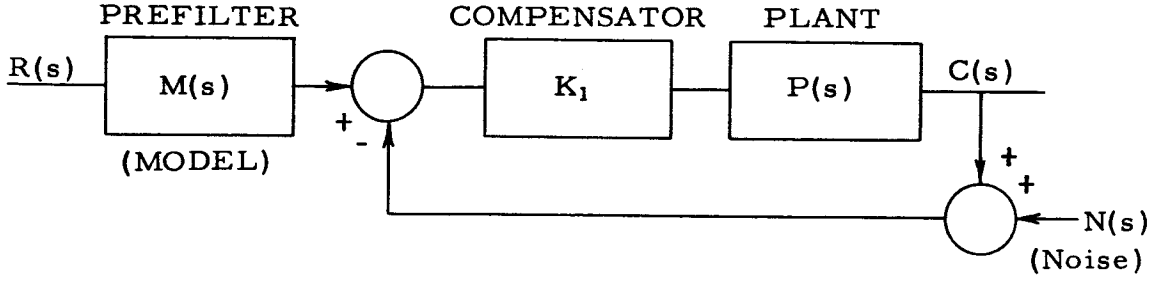

Figure 4. High Gain Compensation With Transducer Noise Input

Degrees-of-Freedom

A plant which has only two access points (the plant input and output points) is termed a two-degree-of-freedom system by Horowitz[2]. The term "two-degree-of-freedom" arises because such systems allow two system functions, such as the system transmission function, T(s), and some disturbance transmission function, to be independently specified.

Since most plants have at least two access points available two-degree-of-freedom design techniques can be used when requirements are specified for only two system functions. Example 1 above demonstrates one situation where only two requirements were made; one on the transmission function, T(s), and one on the elimination of the effect of parameter variations. In general it is possible to conclude that if only two requirements are made in a two-degree-of-freedom system it is not necessary to consider adaptive controls to realize the specifications.

Sensitivity

The concept of sensitivity is used to describe the effect of parameter variations on various system functions. The sensitivity of the function F with respect to a parameter x may be denoted by

$$S_x^F = \frac{x}{F}\,\frac{dF}{dx} = \frac{d \ln F}{d \ln x} \,. \tag{4}$$

That is, the sensitivity is defined as the ratio of the change in the logarithm of F to the change in the logarithm of x. Thus, the sensitivity of F with respect to x indicates the percentage change in F caused by a certain percentage change in x.

Consider the feedback system shown in Figure 5. Assume the

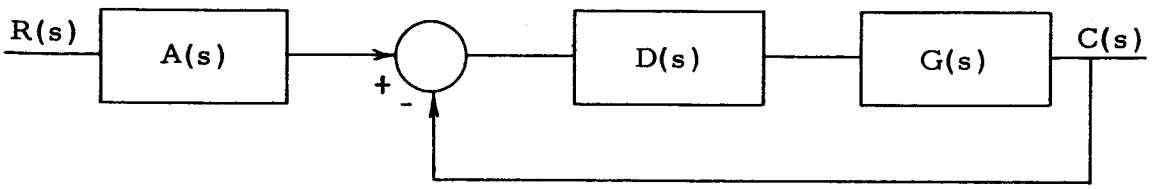

Figure 5. Feedback System

transfer functions A(s) and D(s) to be time invariant. Let the transfer function G(s) contain parameters which may change. The transfer function G(s) may be written

$$G(s) = k \frac{(s + z_1)(s + z_2) \ldots}{(s + p_1)(s + p_2) \ldots} \tag{5}$$

The closed loop transmission function T(s) is given by

$$T(s) = \frac{C(s)}{R(s)} = \frac{A(s)\, D(s)\, G(s)}{1 + D(s)\, G(s)} \,. \tag{6}$$

The sensitivity of T(s) with respect to a variable element x of G(s) is defined by

$$S_x^T(s) = \frac{d \ln T(s)}{d \ln x}$$

$$= \frac{d \ln G(s)}{d \ln x} \quad \frac{1}{1 + D(s)\, G(s)} \tag{7}$$

for example if x is a pole, p_i, of G(s) then (7) becomes

$$S_{p_i}^T(s) = \frac{-p_i}{s + p_i} \quad \frac{1}{1 + D(s)\, G(s)} \tag{8}$$

The sensitivity function is in general a function of the complex frequency s. In most systems it is not possible to keep the sensitivity small for all values of s, therefore, the usual design procedures try to make the sensitivity small in the expected region of operation. However, procedures for doing this are not well developed. The sensitivity function is most useful for small parameter variations and additional study is needed to adequately represent the effects of large parameter variations.

Example 2

In this example the same plant as example 1 will be considered; however, an additional constraint will be added to prevent the high gain technique used in example 1 from working. Again, consider the system shown in Figure 1 with plant parameter variations as shown in Figure 2. Assume it is desired that the transmission function, T(s) be as close as possible to a specified model transfer function, M(s), where

$$M(s) = \frac{1}{s^2 + 1.4s + 1} \tag{9}$$

In addition it will be required that the maximum mean-square value of the plant input, x(t), due to white transducer noise n(t) be limited. Let the mean-square value of x(t) be denoted by MSX. To be specific if N(s) has a unit spectral density it will be required that

$$MSX \leq 0.5 \tag{10}$$

for all plant parameters.

From Figure 1 it can be seen that the noise transmission function from N(s) to X(s) is given by

$$T_n(s) = \frac{X(s)}{N(s)} = -\frac{D(s)\,H(s)}{1 + D(s)\,H(s)\,P(s)} \tag{11}$$

Since N(s) is assumed to be white noise $T_n(s)$ must have at least one more pole than zero or else MSX will be infinite. This requires that the product D(s) H(s) have at least one more pole than zero. Hence, the simplest form of compensation that can be used is to let H(s) = 1 and

$$D(s) = \frac{K_1}{s + a} \quad . \tag{12}$$

The minimization of effects of plant parameter variations require that K_1 and a be as large as possible whereas the constraint on MSX requires that the magnitudes of K_1 and a be limited. The description of the behavior of the system with the compensator can be simplified by defining four different plants (A, B, C, and D) which represent the parameter extremes as indicated in Figure 2. The values of the parameters for these four plants are given in Table I.

TABLE I

Extreme Plant Parameters

Plant	Kp	τ
A	0.5	4.0
B	5.0	4.0
C	0.5	0.5
D	5.0	0.5

The compensator parameters were chosen so that the MSX was satisfied for the four plants. This was done by choosing several positions for the compensator pole, a, and then calculating the maximum value of compensator gain, K_1, which would keep MSX $\leq$ 0.5. The resulting value of K_1 for several values of a along with the MSX for each plant is given in Table II.

TABLE II

MSX for Various Values of Compensator Parameters

		MSX			
a	K_1	Plant A	Plant B	Plant C	Plant D
1	.236	.0307	.5000	.0460	.0290
2	.6873	.1279	.5000	.2070	.1234
5	1.81	.3393	.5000	.4418	.3363
10	2.925	.4340	.5000	.4871	.4331
20	4.35	.4756	.5000	.4977	.4754

It should be noted that the limit was reached for plant B first in each case. If the static gain, which is equal to K_1/a, for the compensator is calculated as given in Table III it can be seen that a maximum in static gain occurs near a = 5.

TABLE III

Static Gain for Compensator Parameters which Satisfy Saturation Constraint

a	K_1	K_1/a
1	.236	.236
2	.6873	.3436
5	1.81	.365
10	2.925	.2925
20	4.35	.2175
40	6.32	.158

Further insight into the behavior the system with this simple compensator may be obtained by studying the step function responses of the closed loop system for various compensator parameters as shown in Figure 6. These transient responses were obtained by setting both the prefilter and feedback element of Figure 1 equal to unity. It may be noted that the response tends to become more sluggish as the compensator pole, a, is moved out. A fairly reasonable response is obtained for a = 5.0 which also gives the largest static gain for the compensator.

The responses shown in Figure 6 only use one degree-of-freedom to satisfy the constraint on MSX. The additional degree-of-freedom may be used to improve the transient response or decrease the effect of parameter variations.

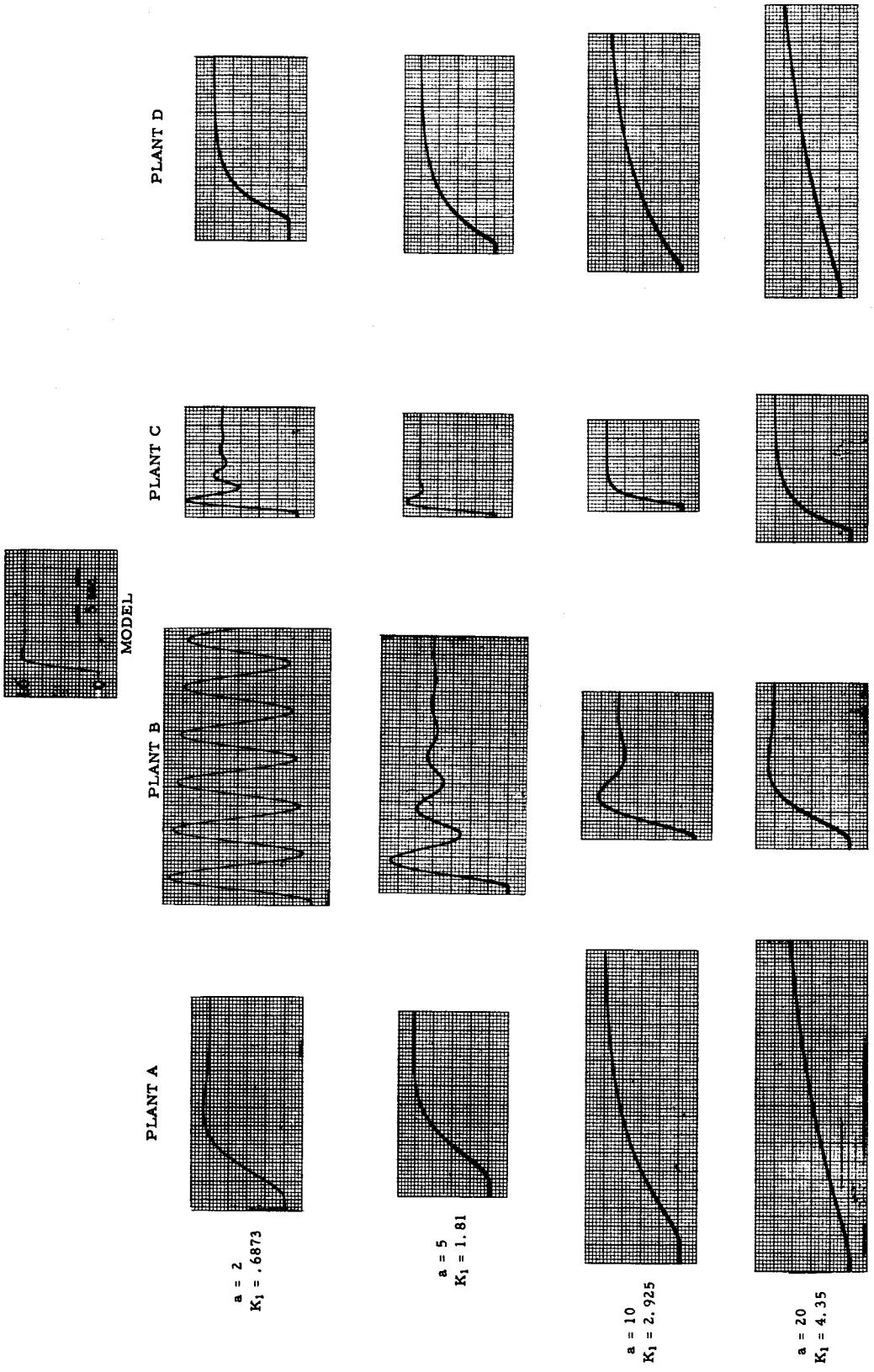

Figure 6. Unit Step Response for System With Various Compensator Parameters

IV. DESCRIPTION OF COMPUTER PROGRAMS

The development of techniques for evaluating system sensitivity, mean-square-value, and frequency response were essential in order to adequately study the behavior of systems with variable parameters. Since much control system analysis deals with functions which are formed from polynomials several Algol procedures for polynomial operations were programmed. These procedures were then used in a driver program to obtain the desired system functions.

Polynomial Operations

Algol procedures were written so that each of the following operations could be performed with a single program statement.

1. READCOEF - this procedure reads the coefficients of an arbitrary sized polynomial. A data card is used to specify the polynomial size and the format to be read. Either exponential or fixed point data may be used. This procedure is used primarily to read in the numerator and denominator polynomials for the various transfer functions.

2. POLYW - this procedure writes the coefficients of any polynomial named.

3. POLYADD - this procedure adds an arbitrary polynomial of degree m to an arbitrary polynomial of degree n.

4. POLYMULT - this procedure multiplies a polynomial of degree m by a polynomial of degree n.

Mean Square Signal Evaluation

In order to evaluate the mean square value of a signal, such as MSX of the above section, a special procedure was written. The two techniques used in this procedure were the tabulated values of integrals given by Newton, Gould and Kaiser,[3] and the matrix form used in the derivation of this table. Two techniques were programmed so they may be used to form a check since the tables are quite complex. Also the tabulated forms are faster to compute for low order systems and the matrix form is useful for higher order systems where the tables do not exist. In the program the tabular form was used for systems through 7th order. The input to the procedure is a ratio of polynomials

representing the signal and the output is a real number representing the mean square value of the signal.

Frequency Response

Procedure FREQ Calculates the magnitude, magnitude in decibels, and phase angle for a transfer function specified as a ratio of polynomials. The calculations are performed for a range of frequencies specified on a data card.

Driver Program

All of the above procedures are used in a driver program to generate various functions of interest in the study. The functions which can be generated include:

1. Closed loop transmission function T(s) which is given by

$$T(s) = \frac{D(s)\ P(s)}{1 + D(s)\ P(s)\ H(s)}$$

2. Sensitivity function which is given by:

$$S(s) = \frac{1}{1 + D(s)\ P(s)\ H(s)}$$

3. Input to the plant due to transducer noise which is given by:

$$X(s) = \frac{N(s)\ D(s)\ H(s)}{1 + D(s)\ H(s)\ P(s)}$$

4. Loop transmission function L(s) which is given by:

$$L(s) = D(s)\ P(s)\ H(s)$$

For each of these systems function either the frequency response or the mean square value or both may be calculated. A program control data card is used to determine which system functions are evaluated. The control card also specified which of the loop transfer functions are to be read in since it is only necessary to read this data if a change is to be made from the coefficients used in a previous run. Results obtained using this program will be described in a separate publication.

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   Two normal-acceleration longitudinal stability-augmentation systems are designed, analog-simulated, and evaluated, for a vehicle having characteristics closely approximating those of the current supersonic transport designs. One system uses the limit-cycle concept and operates on the high-gain principle. The other uses the parameter-perturbation concept and operates on a minimum, mean-square-error principle.

2. Brown, R. R., "A Generalized Computer Procedure for the Design of Optimum Systems -- Part I and II," AIEE Trans. Part I. Communication and Electronics, Vol. 78, July 1959, pp. 285-293.

   The conventional system design procedure is a slow trial and error process by which the best acceptable design produced is not necessarily the optimum one. It also lacks generality, versatility, and in the case of complex systems, accuracy. An improved designing procedure is represented by the gradient methods coded for a digital computer. It consists primarily of a group of criteria for governing the application of gradient minimization procedures. These criteria are selected so as to guarantee convergence to a solution, and to achieve that solution rapidly. Some restrictions on the use of this designing procedure are also given.

3. Calahan, D. A. and M. J. Remec, "Sufficient Conditions for a Hurwitz Polynomical to Remain Hurwitz Under Coefficient Variations," IEEE Trans. on Automatic Control, Vol. AC-9, No. 2, pp. 194-195, (April 1964).

   The test requires knowledge of the position of any dominant roots near the imaginary axis rather than the coefficients of the polynomial.

4. Chang, S. S. L., "Synthesis of Optimum Control Systems," McGraw-Hill, 1961.

Chapter 8 briefly discussed the sensitivity of transient performance on component inaccuracies. Chapter 10 describes self-optimizing systems and Chapter 11 describes stochastic adaptive control.

5. Chen, K., "Analysis and Design of Feedback Systems with Gain and Time-Constant Variations," IRE Trans. on Automatic Control, Vol. AC-6, No. 1, pp. 73-79, (February, 1961). Also published in 1960, IRE WESCON Conv. Record Part 2, pp. 102-108.

Discusses the design of a feedback control system which contains an element with proportional variation of gain and time constant. The stabilization of the system when both the gain and time constant are negative is included.

6. Cruz, J. B., Jr., and W. R. Perkins, "The Sensitivity of General Multivariable Feedback Systems," Report R-227, August 1964. Coordinated Science Laboratory, University of Illinois, Urbana, Illinois. 12 pp. AD-604096.

An approach to the parameter variation problem which is applicable to multivariable systems is proposed. A direct comparison of feedback performance with open-loop performance is used to obtain a sensitivity matrix. This sensitivity matrix provides a basis for designing a multivariable feedback system whose performance is less affected by parameter variations than that for a corresponding open-loop system.

7. Dorf, R. C. and Byars, W. A., "A Modulation Method for Model Reference Adaptive Control Systems," 1963 IEEE International Convention Record, Vol. 11, Part 2, pp. 146-153.

A model reference adaptive control system is described in which a modulation method is used for system probing. The output of the model is modulated and subtracted from the plant output to form an error signal. This error signal is then fed to an error function generator which generates an even function of the input signal, such as, $|e|$ or e^2. The error function signal is demodulated, integrated and filtered. The output of the filter is then used to adjust a system parameter.

This system is claimed to be faster and more accurate than one in which a plant or model parameter is perturbed. The results of an analog simulation using second and third order plants is presented.

8. Douce, J. L. and King, R. E., "A Self-Optimizing Non-linear Control System," Proc. IEE 108B, No. 40, July 1961, pp. 441-448.

A general technique of self-adaptation is presented which adjusts one parameter of a control system to obtain the best response as determined by some built-in optimizing criterion. The method has been applied to a position-control servo-mechanism in which the damping factor is automatically adjusted to give minimum mean-squared error.

It is shown that the introduction of a self-optimizing element effects a substantial improvement in system performance. Experimental results using an analog computer are in good agreement with theoretical predictions.

9. Elgerd, O. I., "Hybrid Computation - A means to Study Predictive Control System Behavior." 1964 IEEE International Convention Record. Vol. 12, Part 1, pp. 30-36.

The author recognized the difficulty of finding optimal control strategies for high order plants. He proposes a "Fast-Model Repetitive Predictor System" (FMRPS) as a technique for attaining a quasi-optimum strategy. In such a system a model controller subjects the "fast-model", a time scaled model of the plant, to exploratory control to predict the future behavior of the actual plant. The control logic provides commands to the real time plant based upon the model response. The commands are on-off in accordance with Pontryagin's Maximum Principle. The author proposes that the control strategy be arrived at by simulation on a dynamic storage analog computer (DYSTAC). The results of the simulation of a simple second order plant are presented and areas for additional research are indicated.

10. Eveleigh, V. W., "Adaptive Control Systems," Electro-Technology, April 1963, pp. 79-98.

A representative set of adaptive-control system examples is given and treated briefly. These include systems using the following control strategies: (a) Holding IRAR (Impulse Response Area Ratio) constant, (b) Peak-Holding optimization, (c) Model Reference Adaptation, (d) A Decoupled Multidimensional System, (e) The Steepest Descent Approach and (f) Multidimensional Incremental Adjustment. Finally, relatively detailed discussions are given to Sinusoidal-Perturbation Adaptive Systems and Signal-Synthesis Adaptive Control.

This paper provides a survey of most of the well-known techniques that have been proposed or developed for adaptive control. Though only a shallow view of present research is given, the paper provides a good survey for people who are interested in learning about the field of adaptive control.

11. Eykhoff, P., "Adaptive and Optimalizing Control Systems," IRE Trans. on Automatic Control, Vol. AC-5, No. 2, pp. 148-151, (June, 1960).

The concept of "odd-function" (error) systems and "even-function" (error) systems is introduced to distinguish between ordinary control systems and adaptive systems. It is concluded that an adaptive system must in some sense learn by making more than one observation and using the resulting information in some optimum manner.

12. Fleischer, P. E., "Optimum Design of Passive-Adaptive Linear Feedback Systems with Varying Plants," IRE Trans. on Automatic Control, Vol. AC-7, March 1962, pp. 117-128.

This paper discusses a procedure whereby the system is designed to be insensitive to plant variations, and have minimum open loop-bandwidth. Some of the procedures to obtain an insensitive system to plant variations resulted in large open loop bandwidth.

Mathematically, the paper discusses how the transfer function $F(s)$ and the change in $F(s)$ with respect to the change in plant parameters $\Delta P(s)$ can be optimally specified with the contradictory requirements given above.

13. Gibson, J. E., "Self-Optimizing or Adaptive Control Systems," Proc. of IFAC, Moscow, 1960, Vol. II, pp. 586-595.

Speed of response and stability of multidimensional adaptive controls are discussed. An ideal multidimensional adaptive control is described. The error criteria used are ITAE and ITSE. The strategy used is to adjust the parameters of a series compensator so as to obtain optimum ITAE or ITSE, using the steepest descent method.

14. Hakimi, S. L. and Cruz, J. B., Jr., "Measures of Sensitivity for Linear Systems with Large Multiple Parameter Variations," IRE Wescon Convention Rec. 2, 1960, pp. 109-115.

Although the paper presents 4 possible sensitivity functions for large parameter variations, and draws attention to a theorem that will give an upper bound to the maximum value of the system function T(s) and a lower bound to the minimum value of T(s), it does not define a sensitivity function for finite multiparameter variation that lends itself to purely analytic approaches. The use of digital computers is widely advocated in this paper as a means of finding the necessary limits on T(s).

The paper also presents a statistical definition of the sensitivity in terms of the standard deviations, of the parameters and the "root means square" of the variation in $T(s)_{s = jw}$. Use of this definition is based on assumed distributions for the varying parameters, with the further assumption that all parameters have the same distribution. Differing distributions among a large number of parameters would make solutions difficult even with computers. A variation of this approach uses the Monte Carlo method for establishing a minimum confidence level for the variation of $T(s)_{s = jw}$. Using these techniques, tolerance levels on the various parameters may be established. In any event practical results seem attainable only with considerable computer implementation, and approaches from the analytic viewpoint are not advanced.

One value of the paper lies in its drawing attention to the Theorem of Myers, giving the limits of T(jw) as a function of the maximum deviations of the parameters. An approach to sensitivity from the mapping direction may be facilitated by further investigation of this Theorem.

15. Horowitz, I. M., "Fundamental Theory of Automatic Linear Feedback Control Systems," IRE Trans. on Automatic Control, Vol. AC-4, No. 3, pp. 5-19 (December 1959).

Describes the basic theory required for the development of a passive adaptive control theory. The reasons for using feedback are reviewed. The beneficial aspects of feedback are quantitatively expressed in sensitivity functions and noise transmission functions. The system with two degrees of freedom is studied in detail. Two methods are presented for the design of a system that will be insensitive to large parameter variations.

16. Horowitz, I. M., "Linear-Adaptive Flight Control Design for Re-Entry Vehicles," IEEE Trans. on Automatic Control, Vol AC-9, No. 1, p. 90-97, (January 1964).

Presents a design procedure suitable for systems with very large parameter variations. The given time domain specifications are translated into approximately equivalent frequency response restrictions to allow a frequency domain design. This results in maximum economy of gain and bandwidth of the system loop transmission. The practicality of the design is discussed in terms of gain and bandwidth demands on the compensating network, the higher order airframe dynamics and the effects of any overdesign on the system saturation tendencies.

17. Horowitz, I. M., "Comparison of Linear Feedback Systems with Self-Oscillating Adaptive Systems," IEEE Trans. on Automatic Control, Vol. AC-9, No. 4, pp. 386-392, (October 1964).

The adaptive and disturbance attenuation properties of a linear feedback system are compared with those of the self-oscillating-adaptive system. For minimum-phase plants, the system sensitivity to feedback transducer noise is used as the basis for comparison.

18. Katayama, A., "Adaptive Control System Design Using Root-Locus," IRE Trans. on Automatic Control, Vol. AC-7, No. 1, pp. 81-83, January 1962 (Correspondence).

This note describes the root-locus approach to the analysis and design of adaptive control systems that contain an element with a variable pole. A technique using the variation on the plant pole to move a compensator pole in the opposite direction is used. This system has the advantage of not attempting direct cancellation. However, a good procedure for the determination of the pole variation is not given.

19. Kaufman, H. and P. M. De Russo, "An Adaptive Predictive Control System for Random Signals," IEEE Trans. on Automatic Control, Vol. AC-9, No. 4, pp. 540-545 (October 1964).

The plant actuating signal is regulated according to the values of the future error and future error rate of a fast time adaptive model. Dual mode control is used consisting of normal bang-bang actuation with linear control introduced for small error and error-rate. No load disturbance or transducer noise is considered.

20. LaBounty, Robert H., "Root Locus Analysis of a High-Gain-Linear System with Variable Coefficients," M.S. Thesis. GSF/EE/64-1. The Air Force Institute of Technology, August 26, 1964, AD-607112.

A technique is developed for applying root locus analysis to high-gain linear systems with variable coefficients. The technique results in a system which can be successfully simulated on an analog computer.

21. Mazer, W. M., "Specification of the Linear Feedback System Sensitivity Function," IRE Trans. on Automatic Control, AC-5, No. 2, pp. 85-93 (June 1960).

The article begins with a review of previous (prior to 1960) work done in the area of sensitivity, and reviews, in greater detail, the use of the sensitivity function, (as defined for a single, slowly varying, plant parameter) according to the "forced response criterion". This method is generally dependent on the type of input used, preferably a number of exponential inputs, and in considering only the forced response this method is of little value in controlling the transient response.

The article then presents a method which for the case of a single, slowly varying parameter is claimed to overcome the shortcomings of previous methods. By use of a mean-squared error technique, which utilizes the power density spectrum of periodic input, the required zeros of the sensitivity function are determined. From a knowledge of these zeros the compensating networks are synthesized. The method has the advantage in that all calculations (the synthesis procedure) takes place entirely in the complex frequency domain. An example is worked out in which the system function T(s) contains a varying gain, K, and hence the percentage change in T(s) is given by S_K^T and computation is thereby facilitated. This result is compared with the corresponding results obtained from the forced response technique, and the results in the time domain are adequately presented.

The technique presented by the paper, does not cover the multi-parameter case. Extension of this technique to the multiparameter case must evidently make use of suitable sensitivity functions.

22. Narendra, K. S. and D. N. Streeter, "An Adaptive Procedure for Controlling Undefined Linear Processes," IEEE Trans. on Automatic Control, Vol. AC-9, No. 4, pp. 545-548 (October 1964).

An adaptive procedure is described which effects a reduction of the mean-square error of a linear stationary random process, without explicit knowledge of the characteristics of the process. The procedure is recursive and, at every step, involves the simultaneous adjustment of an arbitrary number of parameters in a feedback compensator. The adjustment is based on estimates of the error gradient in the space of the adjustable parameters.

23. Perlis, H. J., "The Minimization of Measurement Error in a General Perturbation-Correlation Process Identification System," IEEE Trans. on Automatic Control, Vol AC-9, No. 4, pp. 339-345, (October 1964); Also published in Proc. 1964 JACC, pp. 332-339.

A general identification system using single frequency and multiple-frequency sinusoidal probe signals is studied for a class of time varying processes. It is assumed that the process is nominally known and that the statistical characteristics of its varying parameter and of the environment are known. The identification error is described in terms of the spectral properties of the parameter variations and of the transducer noise. Procedures are given to minimize the perturbation-correlation system's mean-square identification error. This method is especially suited to the identification of slowly-varying systems in the presence of measurement noise.

24. Tiedemen, A. T. and Higgins, T. J., "A Procedure for Systematic Determination of the Effects of Component-value Changes in Automatic Control Systems," Automatic and Remote Controls, J. F. Coales, Editor, Vol. 3, pp. 41-45, Butterworths, 1961.

A description is given of a tabulation in graphical form of the effect of parameter changes on the integral-squared error for some 51 different feedback control system functions. Only 3 graphs are given in this specific paper.

25. Volz, R. A., Optimal Synthesis of Feedback Systems with Parameter Variation, Ph.D. Dissertation, Northwestern University, June 1964.

FINAL REPORT

AN EXAMINATION OF SURFACE STRUCTURES DEVELOPED ON COPPER-NICKEL ALLOYS BY THERMAL ETCHING IN A VACUUM

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SUBMITTED BY:

Dennis O'Neill
Research Metallurgist

William M. Mueller
Professor of Metallurgy and
Head of Metallurgy Department

ABSTRACT

The surface morphologies that result from heating copper-nickel alloys in a vacuum environment were examined by electron microscopy techniques. It was observed that faceting could be produced on alloys of varying composition, but the faceting topography was quite complex and varied with different compositions.

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I. INTRODUCTION

When a metal is heated in certain gaseous or vacuum environments the surface may become rough. This roughening or change in surface structure may appear as grooves at the grain boundaries and as facets on the surfaces of the individual grains. As a rule the facets appear as thin narrow surfaces conforming to low index crystallographic planes. These facets are separated by a complex surface structure which tends to be related to the facets on the low index planes in such a manner that the average orientation of the planes is parallel to the surface of the metal. The phenomenon responsible for the formation of these grooves and facets is termed "thermal etching."

A fundamental problem in the theory of thermal etching is to predict whether a given macroscopic surface will remain flat or break up into facets, and if facets are formed, what orientation they will have. The mechanism for facet formation is not well understood. For many experimental observations it has been assumed that the mechanism for faceting is the result of the minimization of the surface free energy, but other observations support a mechanism of selective evaporation at certain crystallographic planes. Neither mechanism has been able to account for all the observed phenomena resulting from thermal etching, and it is a well documented fact that more experimental work will be required before a clear picture of the faceting mechanism can be presented.

Chalmers, King and Shuttleworth[1] summarized early observations on the phenomenon of thermal etching, and their systematic study of the thermal etching of silver in oxygen, nitrogen, and vacuum initiated many of the later investigations in the field. Recently, Moore[2] has made a compilation of the data available on the faceting of various substances. The following observations on the thermal etching of copper and nickel are reported in Moore's compilation.

When oxygen was present internally either as oxide inclusions or interstitially or as an oxide film, copper exhibited facets of {100} and {110} planes if heated to 950°C in a vacuum of 0.5 Torr. The faceting was attributed to evaporation of an oxide that was selectively formed on particular crystallographic planes. Similar facets were observed in another investigation on spherical crystals of copper that had catalyzed a hydrogen-oxygen reaction, but here it was thought that facets were produced on planes of simple indices as a consequence of the high mobilities of the copper atoms resulting from the reaction.

From observations such as these some investigators have suggested that a low oxygen concentration must be present to produce faceting. However, this seems to be in disagreement with an experiment where facets were produced on oxygen free copper in a vacuum of 10^{-9} Torr.

Very few investigations have been reported in the literature on the faceting behavior of alloys. Since selective evaporation of one constituent may occur during the thermal etching of a multi-component system, it is somewhat more difficult to interpret the faceting in terms of the usual theoretical models; however, investigations of the surface morphologies produced by thermally etching a two phase system may provide new insight for interpreting the mechanism or mechanisms responsible for thermal faceting. With a two phase system the atomic parameters are changed by varying the composition and the other variables such as the oxygen partical pressure, temperature and orientation can be held reasonably constant. The thermal faceting of copper and nickel individually has been studied by many investigators, but no investigations have been reported in the literature on the thermal faceting of copper-nickel alloys.

The object of this investigation was to examine, by means of electron microscopy, the surface morphologies of thermally etched copper-nickel alloys. Several interesting morphologies have been examined and methods are being evaluated for obtaining additional information from these thermally etched surfaces.

II. EXPERIMENTAL TECHNIQUES

A. Metals:

The nickel (Alloy 270) was donated by the Huntington Alloy Products Division of the International Nickel Company, and the limiting composition of this alloy is:

	Percent
Nickel	99.95 min.
Manganese	0.003 max.
Iron	0.005 max.
Silicon	0.003 max.
Sulfur	0.003 max.
Copper	0.003 max.
Cobalt	0.003 max.
Carbon	0.02 max.
Chromium	0.003 max.
Magnesium	0.003 max.
Titanium	0.003 max.

The copper was 99.999 percent pure.

Charges of copper and nickel were prepared by filing all the surfaces of each piece of metal, electropolishing in phosphoric acid and then rinsing in absolute ethyl alcohol. All charges were melted in Coors AD99 alumina crucibles. These crucibles were cleaned with a potassium dichromate-sulfuric acid cleaning solution, rinsed with water and ethyl alcohol and heated in air to 800°C prior to melting the charges.

Several melting methods were tried in order to obtain homogeneous alloys. Charges prepared by induction melting in small alumina crucibles under a vacuum of 5×10^{-5} mm Hg exhibited much surface porosity. Charges prepared by melting small quantities of metal (similar to 20 grams) in an inert gas, non-consumable electrode, arc furnace did not appear to be homogeneous throughout as determined by optical examination. These same charges were remelted with induction heating using a tantalum susceptor around the crucible and under a dry argon atmosphere. The resulting melts appeared homogeneous but were rather fine grained.

The strain-anneal method for producing large grained specimens of the various copper-nickel alloys was not appropriate because of the limited amount of each composition that was being used and because of the numerous deviating orientations in the form of twins that are produced during the process. Copper single crystals and large grained alloy specimens were successfully produced by using a modified Bridgman solidification method where an alumina boat was pulled through the natural temperature gradient of a horizontal tube furnace in the vacuum system shown in Figure 1.

B. Surface Preparation

Small specimens with a cross section of about 6 mm by 6 mm were cut from the various alloy compositions with a jeweler's saw. For thermal etching studies, each specimen was then mounted in Koldmount, self-curing resin. Microsection of the specimens were prepared by grinding on a series of silicon carbide abrasive papers, rough polishing on 6 micron diamond abrasive and final polishing on 1 micron diamond abrasive. Specimens were easily removed from the self-curing resin by heating on a hot plate. The specimens were then cleaned by electropolishing in a 1:1 phosphoric acid-methyl alcohol electrolyte and rinsed in absolute ethyl alcohol.

On some of the specimens it was desirable to polish one surface to a specific crystallographic orientation. To accomplish this an X-ray goniometer was modified to fit on an electro-mechanical polishing apparatus as shown in Figure 2. The vertical wheel on this polisher rotates at about 50 rpm and the goniometer rotates in the same direction at about 200 rpm. The specimen is attached to the metal pedestal of the goniometer by means of a mixture of powdered aluminum in Duco cement. After the mixture dries, the sides of the pedestal and specimen are coated with Microstop stop-off lacquer to prevent chemical attack of the mixture by the electrolyte. When the speciemn surface has been polished flat, the goniometer with attached specimen is placed on a modified Unicam X-ray camera, and the crystallographic orientation of the surface is determined from back reflection Laue photographs.

C. Thermal Etching

The first specimens were thermally etched in either a vertical or horizontal tunsten wound tube furnace. The entire furnace assembly was placed in the vacuum system shown in Figure 1. With either

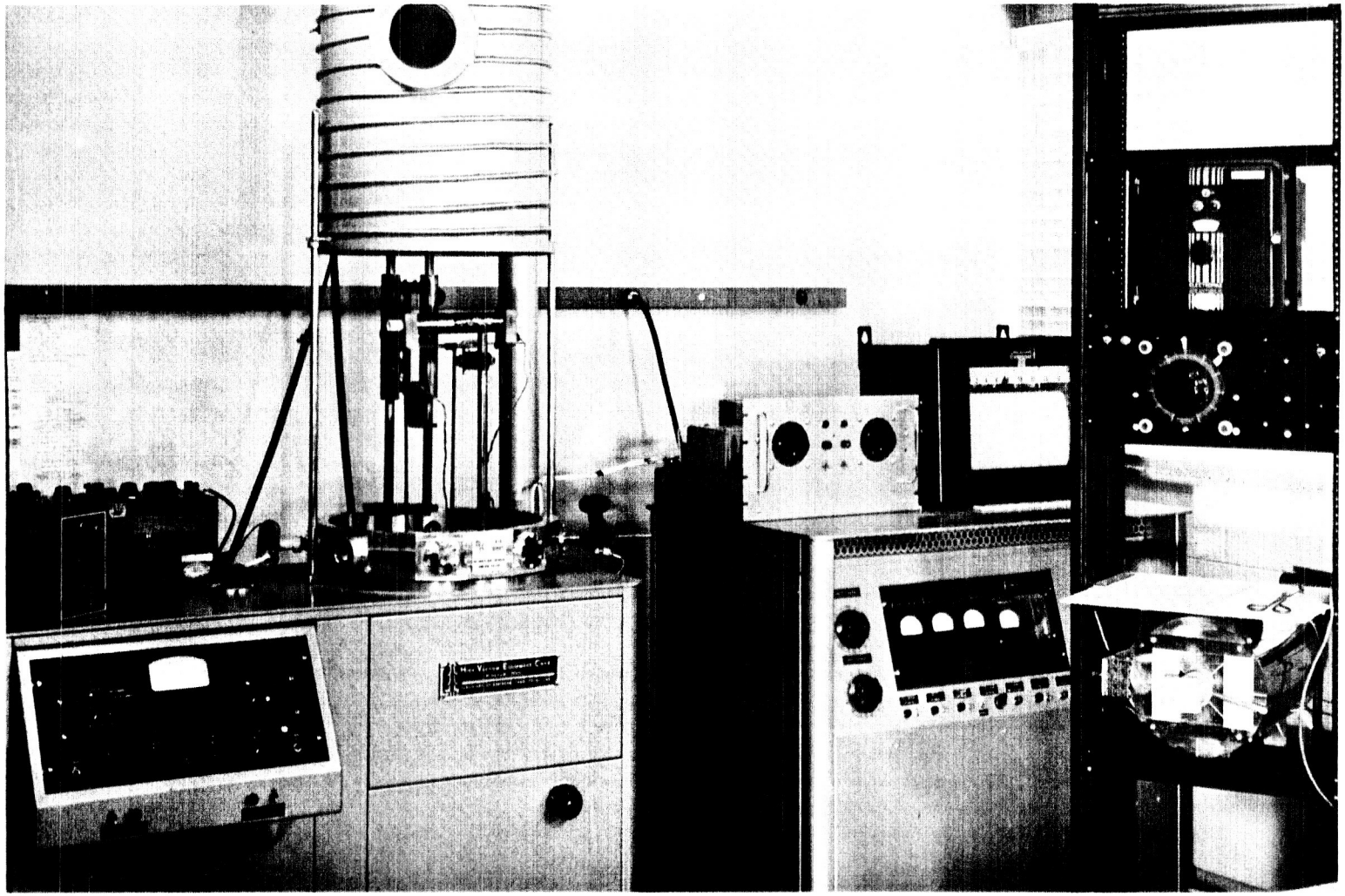

Figure 1. Vacuum System for Producing Large Grained Alloy and Single Crystal Copper Specimens

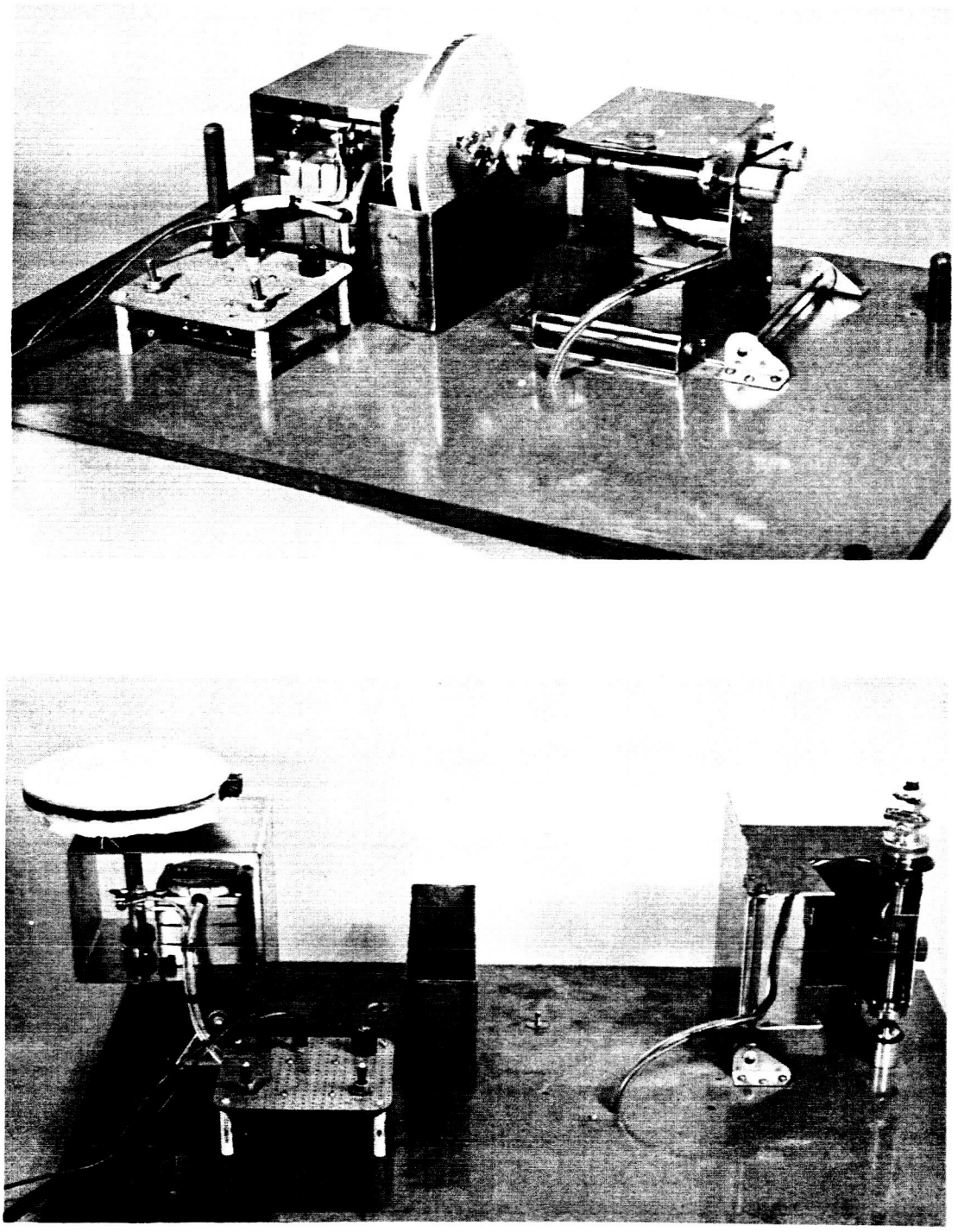

Figure 2. Electro-Mechanical Polishing Apparatus. Top--in operating position. Bottom--in position for removing electrolyte and goniometer.

furnace arrangement it was difficult to obtain accurate temperature measurements and the surface of several of the thermally etched specimens became contaminated. This contamination was thought to have been in part the result of decomposition of the lavite furnace tube supports. In order to overcome some of the difficulties encountered with these furnace arrangements, use was made of the vacuum system shown in Figure 3. The furnace for the system consists of a vertically supported cylindrical tungsten filament surrounded with three concentric tantalum heat shields. The furnace assembly is enclosed in a water cooled vacuum chamber. A temperature controller was connected to the electrical circuitry of the filament in such a manner that temperature variations could be maintained to within ±5°C during a thermal etching run. For thermal etching the specimen was placed in an alumina (Coors AD99) crucible placed in the center of the cylindrical tungsten filament and above a platinum-platinum 13% rhodium thermocouple. A vacuum of about 5×10^{-5} mm Hg was maintained during the thermal etching runs.

D. Electron Microscopy

The thermally etched specimens were too rough for detailed optical examinations, but by using the electron microscope with its inherent high magnification and large depth of focus it was possible to resolve both the coarse and fine details on the etched surfaces.

A two stage replicating method was employed so that the specimens could be retained for further use. The first stage consists of making a plastic replica of the specimen surface. For the second stage, the plastic replica was shadowed with a platinum-carbon alloy at an incident angle of 45° with the replica surface, and then carbon was vertically evaporated on the replica. Replicas of the faceted types of surface morphology were quite prone to tearing during the process of removing the plastic from the carbon replicas. This tearing was decreased by rotating the plastic replica while the carbon was being evaporated.

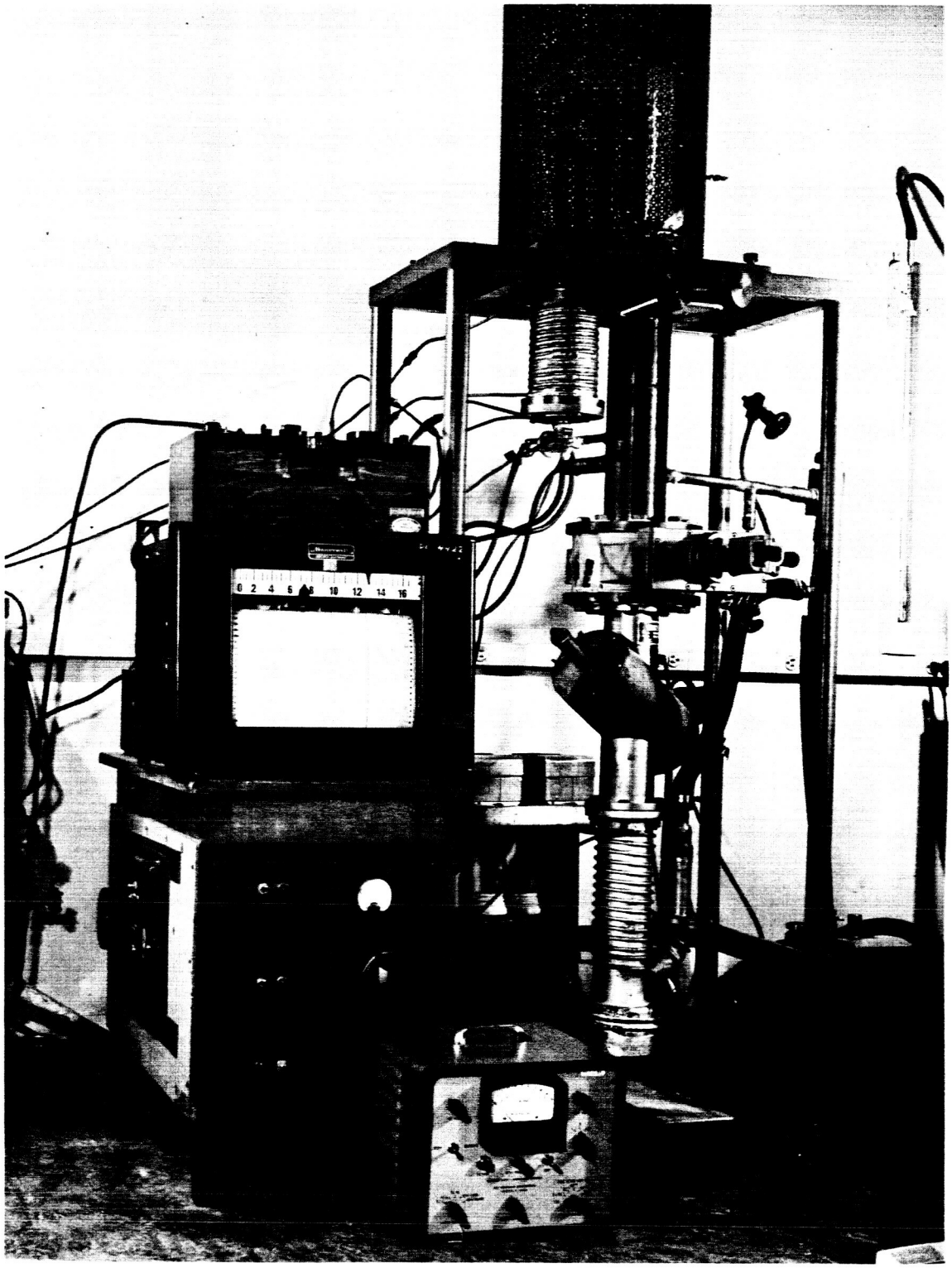

Figure 3. Vacuum System Used for Thermal Etching

III. EXPERIMENTAL RESULTS

The examination of many thermally etched surfaces on copper-nickel alloys indicates that many factors such as temperature, pressure, orientation of the polished surface relative to the crystallographic orientation and composition of the alloy all affected the faceting morphology. Table 1 lists experimental conditions for some of the thermal etching runs conducted during this investigation.

Copper specimens were etched at 1000°C or 83°C below the melting point so that the faceting behavior could be correlated with results of other investigators.[2,3] The etching temperature for nickel (Run 10) was also selected at about 83°C below the melting point of nickel, and the temperature (1185°C) for etching the 50 wt.% copper-50 wt.% nickel alloy (Run 20) was midway between the etching temperature of the copper and the nickel. For a few compositions, two different etching temperatures were used, but the faceting results do not show any special trends for making predictions on how the faceting behavior changes with temperature.

Copper specimens were etched under different vacuum conditions, and the large terrace type of faceting seemed to predominate with a poorer vacuum. A copper specimen etched in a covered alumina crucible exhibited a smoother surface and a much finer scale of faceting than did one that was etched in an open crucible under the same experimental conditions.

Figure 4 depicts a copper single crystal that was etched (Run 6) in a poor vacuum (2×10^{-2} mm of Hg) at about 900°C. The large terrace-like areas are crystallographic planes of a low index and the rough narrow surfaces adjoining the terraces represent a complex plane which is usually thought to be made up of several planes of low indices. The rough surfaces partially surrounding the faceted portion of the crystal are oxide crystals that were produced during etching.

The micrograph shown in Figure 5 represents the etched surface of a copper single crystal (Run 19). Prior to etching the surface of the specimen was polished so that it was parallel to the {110} set of crystallographic planes. Three distinct surfaces are developed in this micrograph. The rectangular surfaces represent the {110} set of planes, and the surfaces inclined at an angle to these but having a common edge correspond to the {111} planes. The surfaces on the right hand side of the micrograph represent the {100} set of planes.

TABLE 1

Experimental Conditions for Thermal Etching

Composition (wt. percent)	Run No.	Temperature (°C)	Time (Hours)	Vacuum (mm of Hg)	Remarks of Optical Examination
Copper-single crystal	3	1000	40	5×10^{-5}	Many pits; no facets--polished surface almost parallel to {100}
Copper-single crystal	5	1000?	24	2×10^{-2}	Many large facets--polished surface almost parallel to {100}
Copper-single crystal	6	900?	20	2×10^{-2}	Large facets surrounded by oxide crystals
Copper-single crystal	19	1000	50	2×10^{-5}	Shows {100}, {110} and {111} surfaces--polished surface parallel to {110}
Copper-polycrystalline	14	1000	48	5×10^{-5}	Many large pits; some pits show faceting--crucible covered during run
Copper-polycrystalline	17	1000	50	5×10^{-5}	Many large pits with faceting in and around pits
50 copper-50 nickel polycrystalline	7	970	50	5×10^{-5}	Many pits; no facets.
50-copper-50 nickel polycrystalline	20	1185	50	5×10^{-5}	Numerous pits; no facets.

TABLE 1 (Cont.)

Composition (wt. percent)	Run No.	Temperature (°C)	Time (Hours)	Vacuum (mm of Hg)	Remarks of Optical Examination
16 copper-84 nickel polycrystalline	11	1295	50	5×10^{-5}	Large pits and facets which exhibit four-fold symmetry.
16 copper-84 nickel polycrystalline	18	1000	50	5×10^{-5}	Very small pits which are not uniformly separated.
Nickel-polycrystalline	9	1200	50	5×10^{-5}	Faceting on certain grains.
Nickel-polycrystalline	10	1370	50	5×10^{-5}	Fine scale faceting.

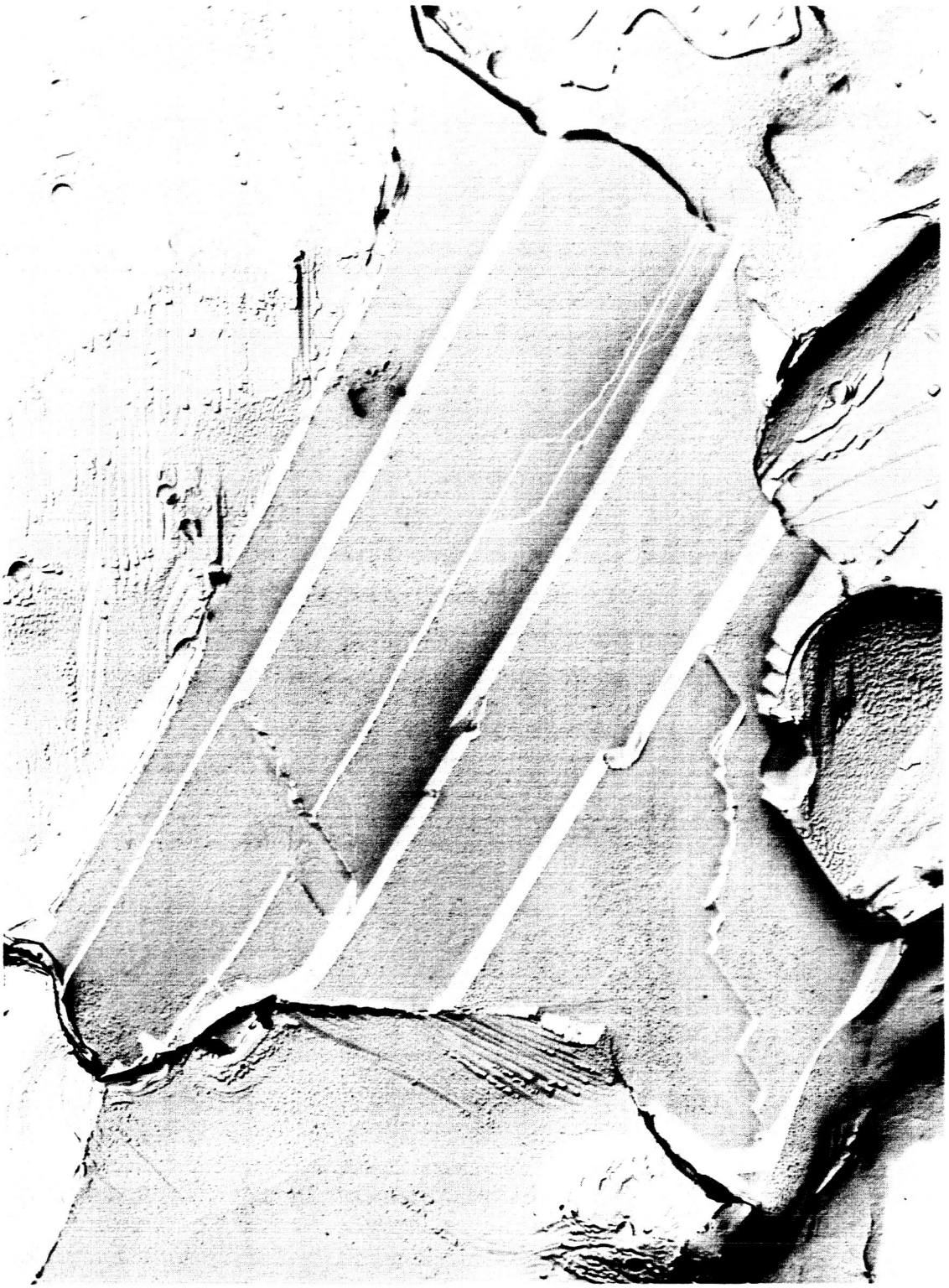

Figure 4. Electron Micrograph of Thermally Etched Copper Single Crystal. 9,600X.

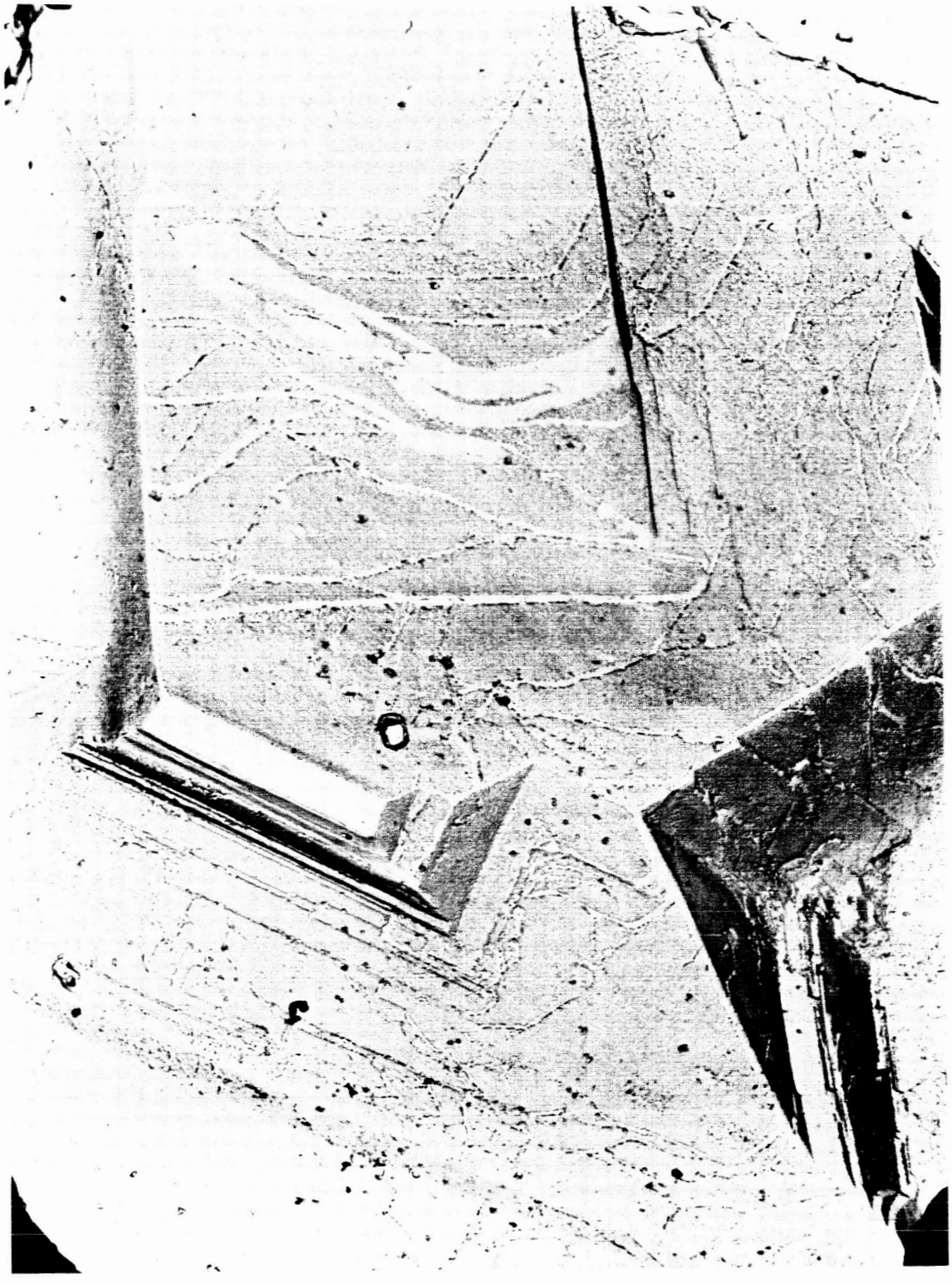

Figure 5. Electron Micrograph of a Faceted Copper Single Crystal Polished Parallel to the {110} Planes. 5,500X.

Rhead and Mykura[4] have observed a similar type of faceting on silver when it was heated in a flow of air to enhance evaporation, and it was thought that evaporation plays an important role when facets are produced which make relatively large angles with the original surface.

No faceting was observed by electron microscope examination of the 50 wt. % copper-50 wt. % nickel alloy etched at 1185°C (Run 20), but the resulting surface appeared very rough. A typical micrograph of the many large shallow pits on this etched alloy is shown in Figure 6. A previous run (Run 7) on an alloy of this same composition exhibited a very fine scale faceting when etched at a temperature of 970°C. An electron micrograph of this fine scale faceting is shown in Figure 7.

Figures 8 through 11 depict the surface morphology of a 16 wt. % copper-84 wt. % nickel alloy that was etched at 1295°C (Run 11). The surface of this specimen shows numerous large pits and faceting occurs both in the pits and on the surface. This faceting in the pits nicely illustrates the cubic symmetry of the alloy. The development of large high angle facets in these pits might indicate that an evaporative mechanism rather than one of minimum surface free energy is responsible for the faceting topography, but on this basis it is difficult to explain why the whole surface does not "break-up" into high angle facets.

Figure 12 is an electron micrograph of the same specimen as shown in Figures 8 through 11, but it was etched at 1000°C (Run 18). Note the small randomly scattered pits that do not show any faceting.

Figure 13 shows the faceted surface of nickel at 1370°C (Run 10). From close examination of this micrograph one can conclude that the surface is composed of three facets. Two are perfectly planar and probably represent low index orientations whereas the other is for the most part non-planar. This non-planar facet is sometimes referred to as the "gable end."[4] Faceting of this type has been observed on silver[4] and copper[5], and the equilibrium of such a surface can be evaluated in terms of the surface free energy of the three facets where they meet to form a pyramid. Two faces of the pyramid represent the planar faces or planes of known orientation; hence, equilibrium will depend on the orientation of the non-planar or "gable-end" orientation.

Figure 6. Electron Micrograph of a Thermally Etched 50 wt. % Copper-50 wt. % Nickel Alloy. 6,630X.

Figure 7. Electron Micrograph of a Thermally Etched 50 wt. % Copper-50 wt. % Nickel Alloy. 52, 000X.

Figure 8. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 5,500X.

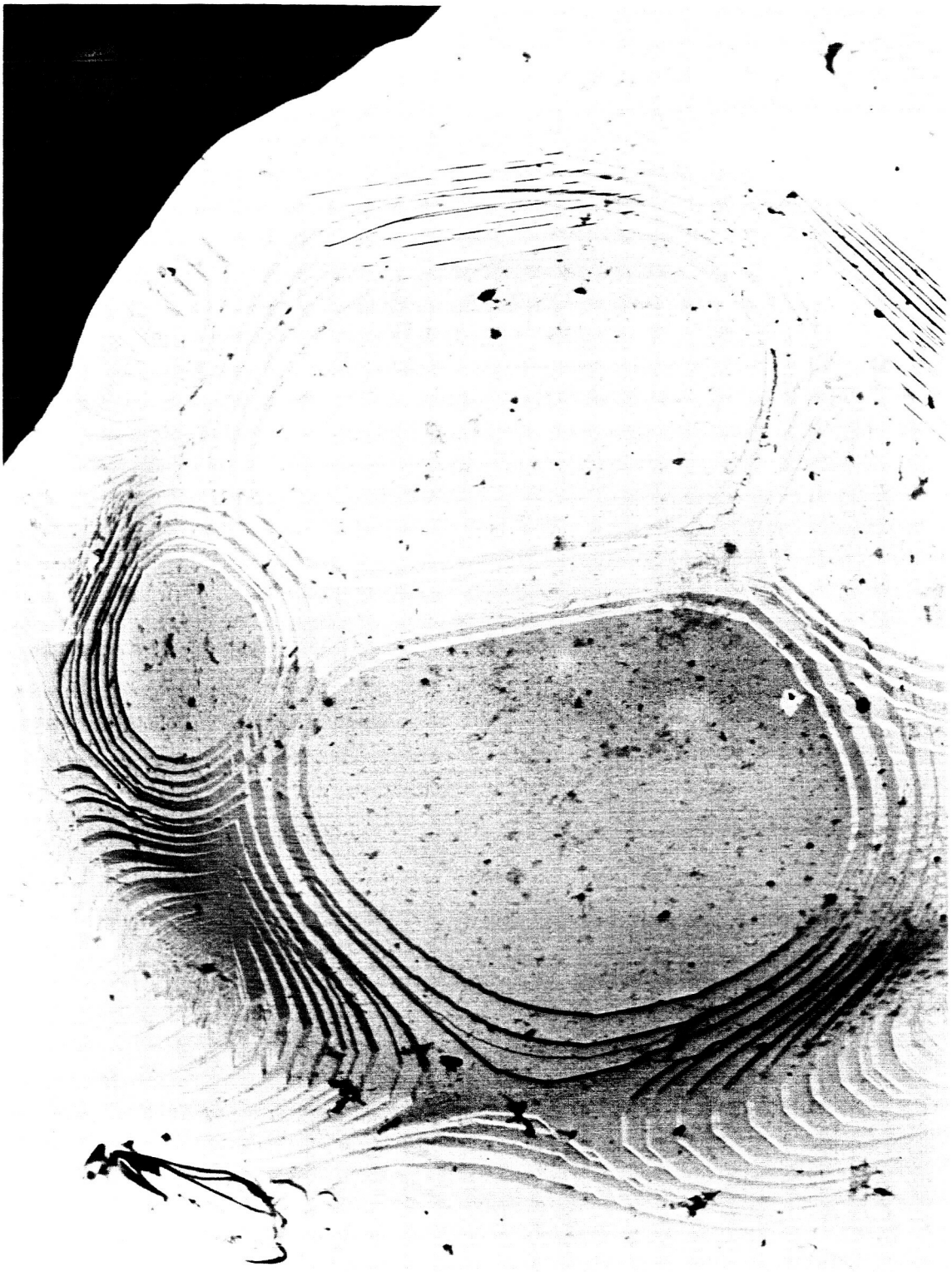

Figure 9. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 5,500X.

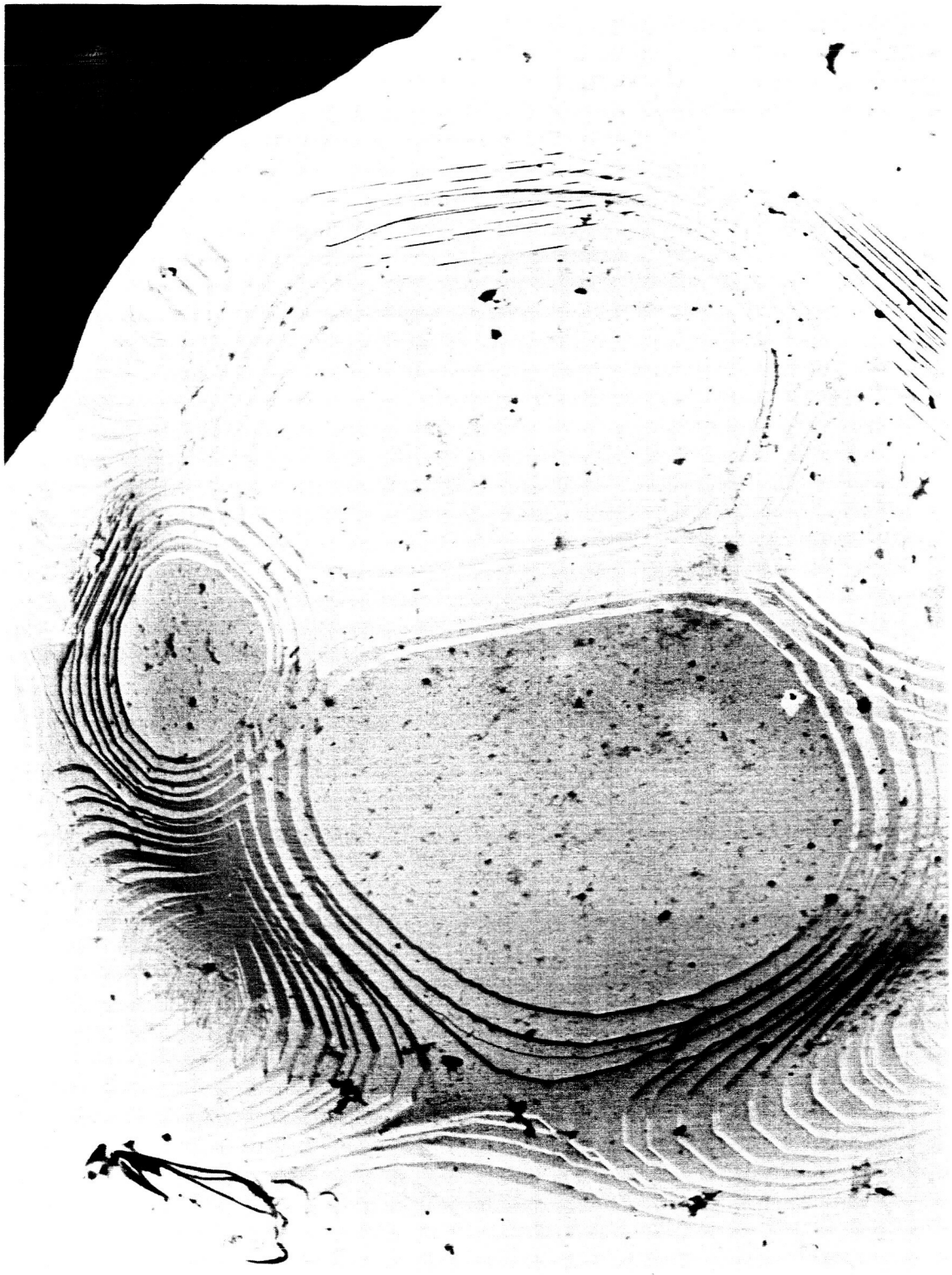

Figure 9. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 5, 500X.

Figure 10. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 5, 500X.

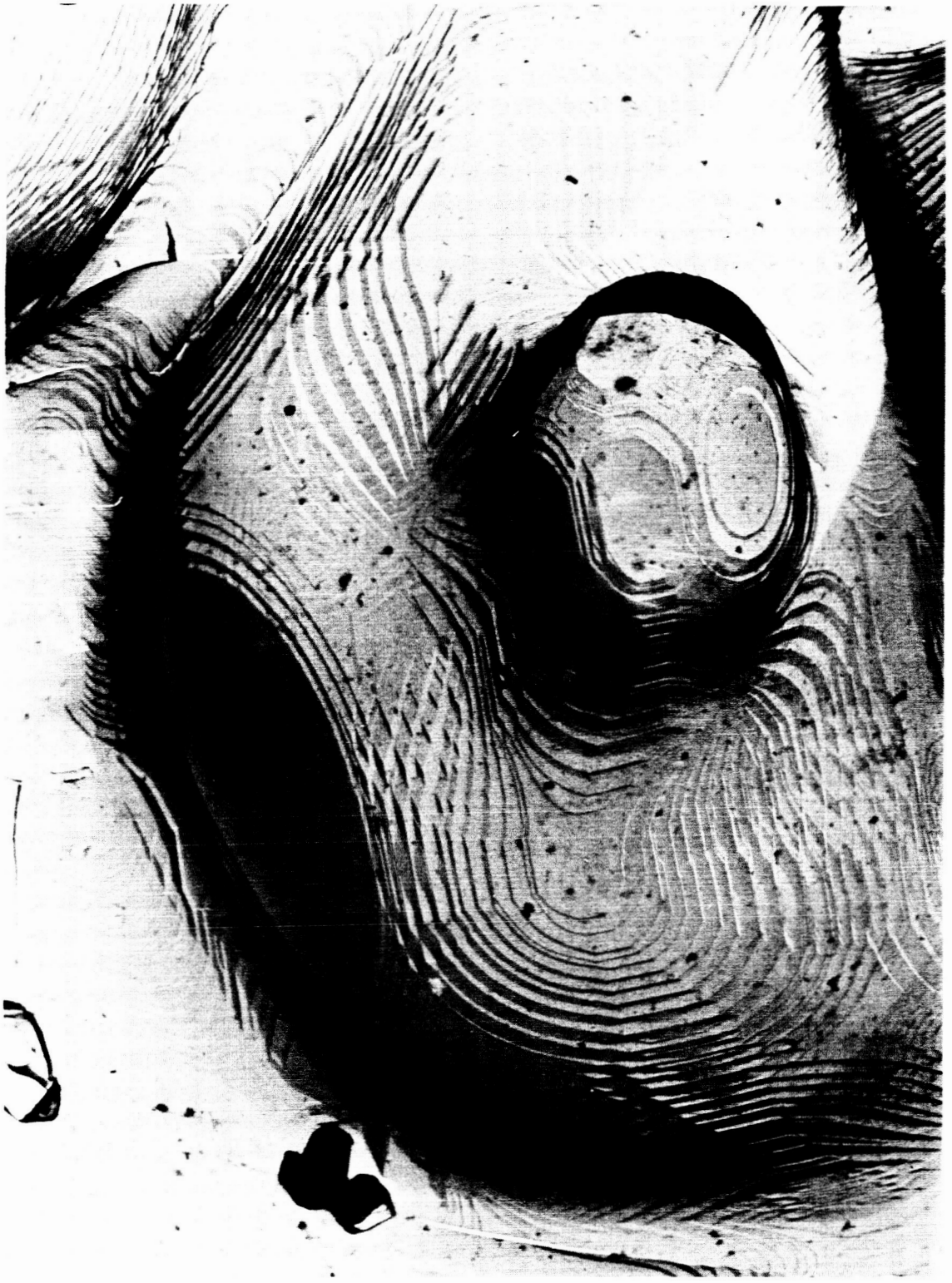

Figure 11. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 5, 500X.

Figure 12. Electron Micrograph of a Thermally Etched 16 wt. % Copper-84 wt. % Nickel Alloy. 21,200X.

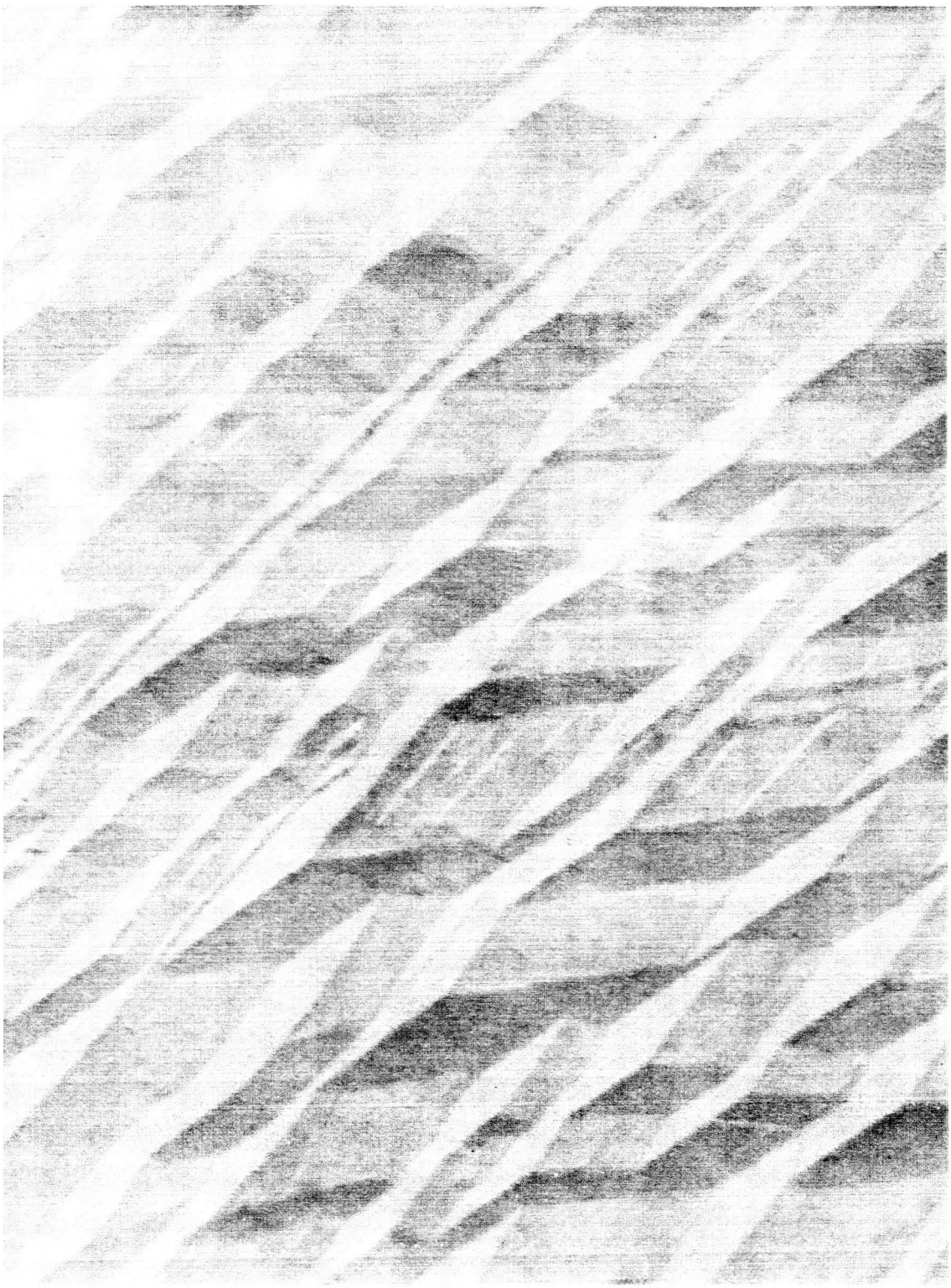

Figure 13. Electron Micrograph of Thermally Etched Nickel. 37,500X.

IV. SUMMARY

Faceting usually occurs under restrictive conditions of pressure, temperature and chemical reactivity with the environment. During this investigation several copper-nickel alloys have been thermally faceted in a vacuum of 5×10^{-5} mm of Hg. The faceting morphology varied considerably from composition to composition. The fact that faceting did occur on all copper-nickel alloys under the given experimental conditions is of significance for conducting additional investigations in this area. It is now possible to hold all experimental parameters except composition constant while the geometry of the facets is studied as a function of composition.

This research on thermal etching is being continued and will be used by Mr. O'Neill as partial fulfillment of the requirements for the Degree of Doctor of Philosophy. Upon completion of the dissertation for this degree, which will include the work covered in this report, the results will be submitted for publication in a scientific journal. Tentatively, ideas are being formulated for writing a research proposal to investigate the thermal faceting of alloys under ultra high vacuum conditions.

V. ACKNOWLEDGMENTS

The authors wish to thank Dr. Monte J. Pool for his helpful suggestions and criticism.

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FINAL REPORT

A SURVEY OF AVAILABLE DIGITAL COMPUTER PROCEDURES FOR INVERTING AND FINDING THE EIGENVALUES AND EIGENVECTORS OF LARGE MATRICES WITH ADAPTATIONS FOR CURRENT STRUCTURAL RESEARCH

A Research Project Supported by NASA
Grant in the Space-Related Sciences

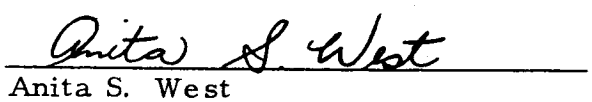
NsG-518

Project No. DRI-618

University of Denver

June 1965

SUBMITTED BY:



Anita S. West
Research Mathematician
Mechanics Division

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ABSTRACT

The partial differential equations of motion of shell structures for aerospace applications subject to arbitrary loads may be extremely difficult or even impossible to solve. Since the digital computer is now an available tool for the structural engineer, current research has been directed towards methods which involve matrix formulation of large systems of algebraic equations and these require rapid and accurate computer solutions. Recognizing the accuracy problems inherent in working with large matrices, this study has been undertaken to survey the available computer programs for large matrix inversions, and for eigenvalue and - vector solutions; to check out these programs and translate, where necessary, for the Burroughs B5500 computer, thus providing a handbook of program input information and at the same time recommending techniques for using these programs most efficiently for structural applications.

I. INTRODUCTION

A great need exists for the rational design of shell structures because of their inherent structural and economic advantages. Solution of the differential equations of equilibrium of shells for even static loads are extremely complex. Mathematical difficulties increase considerably in the case of dynamic loads, suddenly applied loads, arbitrary cross sections, etc., until they reach the point where solutions may be prohibitive or even impossible. Now that digital computers are an everyday tool for the design engineer, there has been a renewed interest in the direction of methods of analysis which involve matrix formulation of algebraic equations and matrix solutions for discrete elements rather than the solution of the partial differential equations. Current research in the field of structural analysis, as well as in elastic stability investigations, are requiring accurate and rapid solutions with very large matrices.

This study has been undertaken to make existing computer programs (in Fortran as well as Algol) available at the University of Denver Computer Center to facilitate future research. Another objective of the study is to determine the maximum matrix sizes for which these programs give acceptable accuracy and to pinpoint the areas of future program needs. The procedures investigated in this study were used in master programs for typical structural problems, and the driver programs are written with the appropriate options.

The programs presented in this report compute the inverse and the eigenvalues of symmetric matrices and the inversion of a non-symmetric matrix. In addition, an original subroutine is included for obtaining improved accuracy in the inversion process by matrix iteration. Instructions are also included for partitioning large matrices in the event machine storage is inadequate.

One additional routine is included here for the purpose of demonstrating the compilation of a large matrix (90×90) without tediously computing and inputting each of the 8100 elements. The compilation is, of course, valid for only the example problem, but the example demonstrates the manner in which many large matrices may be compiled on the computer.

A list of additional selected programs available in the Denver area for solutions of eigenvalues and vectors and inversions of non-symmetric matrices together with summary descriptions are included in the Appendix.

II. COMMENTS ON MATHEMATICAL PROBLEMS INHERENT TO LARGE MATRICES

The algebraic manipulation of matrices and matrix equations presents no problem for the solution of all the elementary operations as well as for characteristic or eigen-numbers and vectors. The methods of solution are numerous and well-expounded in the literature, and computer programs are plentiful.

Many of these methods falter, however, when the matrix is of large order, say $n > 100$. Computational problems are influenced not only by the size of the matrix, but by other considerations, including symmetry, the behavior of the array; that is, the comparative order of magnitude of the elements and how they are positioned in respect to the main diagonal, the density of the matrix, etc.

Reduction techniques, elimination methods, triangular factoring, diagonalization and all the refinements of these methods for finding a matrix inverse are subject to large errors because of simple round-off. Two methods customarily used to reduce this error are column scaling (not suitable for all matrices) and the use of double-precision computer arithmetic, which more than doubles the significant digits of each number but necessitates the use of subroutines which increase computation time on the order of five to ten times, a prohibitively high price for most applications. In addition, valuable machine storage is lost.

The direct methods (non-iterative) of matrix inversion are generally recognized to be well suited to computer techniques because they permit the reduction of a matrix, $[A]$, to an array which can be saved for use at any time for solution of the matrix equation, $[A]\{X\} = \{B\}$ with different right-hand sides. In order to avoid slow iterative refinements, there is a real need for error analysis and the choice of computational methods which minimize the errors that are intrinsic to the computations in solving the problem of the general matrix of large order.

The alternative Monte Carlo methods provide a simple computational approach to the statistical estimation of the elements of the inverse which are not affected substantially by round-off and truncation error, but the statistical variation of the results tends to be quite large in most cases until refined by many additional random walks. Therefore, the technique is most widely used for obtaining rough

estimates very quickly, and for single column inversions, useful for point loads. An iterative process for improving the inverted matrix is useful and allows the inverted matrix to be computed to as high a degree of accuracy as is required, but for very large matrices computer time for handling the necessary matrix subtractions and multiplications may be extremely costly. An original matrix iteration subroutine is given in the Appendix and can be used as a procedure with the inversion programs documented here. Partitioning techniques are widely used for large matrices. For a non-definite and sparse matrix the problem of selecting a square sub-matrix of useful size whose determinant is non-vanishing may be a problem. In any case, the computer operations are many and long and this is usually done as a last resort. Full instructions for partitioning large matrices for inversion are also included in the Appendix.

The mathematical methods for determining the eigenvalues and vectors (modes and modal shapes of free vibration) of a matrix are equally well treated in the literature. Those methods which are specifically for real symmetrical coefficient matrices are surveyed here since structural applications very often yield matrices of this type, and the solution is simplified greatly by this fact. A real symmetric matrix guarantees real eigenvalues and a set of eigenvectors which are orthogonal. This means that a reduced matrix may be used to compute the vectors once the eigenvalues are determined, which is far more efficient than solving the set of equations produced by the input matrix. Despite these savings, there are still storage and accuracy problems connected with these solutions and computer time becomes a significant factor in influencing the choice of method. Obviously an iterative procedure to refine the eigenvalue solution is extremely useful. On the other hand, completely iterative methods, such as the Stodola and Vianelli, are so time consuming that their primary use is in solving for one or two critical values with excellent accuracy. It becomes a matter of judgment then to decide at what point the optimum balance between accuracy and computer time is reached.

The two most widely used methods for finding the eigenvalues or characteristic roots of a real symmetric matrix are those attributed to C. G. J. Jacobi and that of W. Givens, based largely on the Householder method with appropriate modifications for high speed computers.

The Jacobi method appears to be most efficiently used as it was revived by J. von Neumann. It is a well known mathematical fact that if an orthogonal matrix [S] has been found which transforms a real

symmetric matrix [A] into a diagonal matrix [D] , then the i^{th} diagnol element of [D] may be adopted as the i^{th} eigenvalue of [A]. The problem then, is to find [S]. The fundamental approach of Jacobi is to annihilate, in turn, selected off diagonal elements of [A] by elementary orthogonal transformations (trigonometric substitutions). This portion of the Jacobi method is an iterative procedure. Pope and Tompkins have made modifications to the Jacobi technique to speed up the solution. They examine each pivotal or off-diagonal "candidate" in regular sequence and perform the transformation only if the magnitude of the pivotal element exceeds a certain value. The process is convergent for all real symmetric matrices. Further, results due to Goldstine, Murray and von Neumann show that the Jacobi method is stable against round-off error. A computer program by Y. Bard follows this method quite closely.

The first step in the Givens method is the reduction of the real symmetric matrix [A] to tridiagonal form, [T] . For the reduction Householder's method is used. Following the reduction, the leading principal minors of [T] form a Sturm sequence and this result can be used to obtain accurate approximations to the eigenvalues of [A]. This is accomplished by successive bisections of intervals in which the Sturm sequence indicates an eigenvalue exists. The Wilkenson method solves for the eigenvectors of the reduced method and transforms them for the solution to the input matrix [A]. A SHARE program available in FORTRAN II and IV with appropriate subroutines for the Givens method has been written at the University of California.

The method or combination of methods chosen for solutions should, of course, depend upon the application, but should also be best suited to the particular computer on which the program will be primarily used. Most of the programs described in this report give satisfactory results for general matrices of order less than 50 but give good results for larger matrices only with ideal matrix conditioning. More specifics regarding accuracy are discussed separately in the program descriptions.

III. COMPILING A LARGE MATRIX ON THE COMPUTER

Compiling large matrices and inputting these problems for the computer are, in themselves, time consuming and error producing chores. When working with large matrices the computer should be instrumented as soon as possible to handle this portion of the problem. For instance, when compiling the matrix of stiffness elements for a plate problem, the pattern for computing the elements was quickly established. The following example from the thesis problem of J. Shaver (Reference 5), demonstrates the automatic compilation of a 90 × 90 matrix and produces the compiled matrix on punched cards in a manner compatible with procedures for future matrix operations. If there were no need to preserve the compiled matrix on cards the punching option could be omitted and the desired procedure called directly, with merely a printed matrix written for future reference and as a programming check.

Example: Consider a square plate of uniform cross section with constant material properties fixed on three sides with the fourth edge free.

The matrix is compiled of forces due to unit motions at each of the numbered positions. The element A [I, J] refers to a force at I produced by a unit motion at J. A [I, J] = A [J, I] due to a well known reciprocity relation, therefore the matrix is symmetrical, requiring that only one half need be compiled. After compilation the program fills the lower half of the matrix with computed values from the upper half. Two 6 × 6 matrices were quickly established for the plate. The first of these for forces at 1, 2, 3, 4, 5 & 6 is valid across the entire plate through 85,

	1	2	3	4	5	6
1	4. 32		4. 32	-4. 32		43. 2
2	- - - - -	12. 0			-12. 0	
3	- - - - - - - - - - -		576. 0		-43. 2	288. 0
4	- - - - - - - - - - - - - - - - - -			4. 32		-43. 2
5	- -				12. 0	
6	- -					576. 0

86, 87, 88, 89 and 90. Likewise a second matrix

ASSEMBLING A LARGE MATRIX ON THE COMPUTER

Example: Numbering System for Matrix of Stiffness Elements for Square Plate

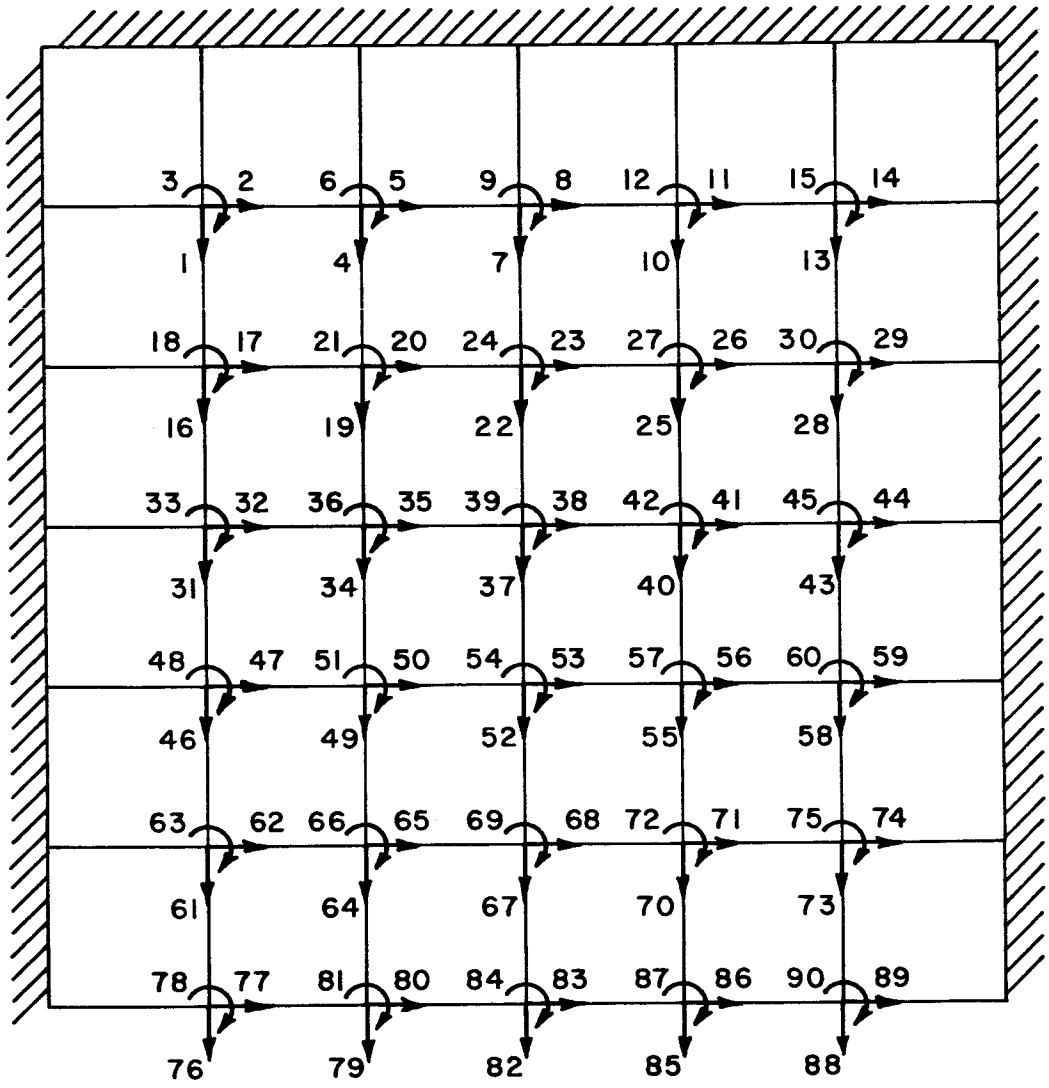

Figure 1. From "Matrix Analysis of Cylindrical Shell" Unpublished Thesis, James Shaver, University of Denver

	1	2	3	16	17	18
1	12.0			-12.0		
2	- - - - - -	-4.32	43.2		-43.2	43.2
3	- - - - - - - - - - - -		576.0		-43.2	288.0
16	- - - - - - - - - - - - - - - - - - - -			12.0		
17	- -				-4.32	-43.2
18	- -					-576.0

produces input for all forces through those numbered 73, 74, 75, 88, 89 and 90. The following program listing produced the entire matrix, adding components algebraically wherever necessary, and printing and punching the resulting compiled matrix, with a savings of several hours of hand calculations, program inputting and key punching time.

```
DENVER, COLORADO,  MAY 12, 1965

                    COPY OPTION  =  OMNI

COMMENT   MATRIX COMPILE SAMPLE PROGRAM    A. WEST;
          BEGIN
INTEGER         P;
LIST            ORDER(P);
FORMAT IN       FIN1(I4);
FILE IN         CARD(2,10);
FILE OUT        PUNCH 0(2,10);
FILE OUT        PRINT 4(2,15);
                READ (CARD,FIN1,ORDER);
          BEGIN
INTEGER         I,J,K,L,M,N,TEST;
ARRAY           A[0:P,0:P];
LIST            MATRIN(I,FOR J=1 STEP 1 UNTIL P DO [J,A[I,J]]);
LIST            LIST2(FOR J =1 STEP 1 UNTIL P DO A[I,J]);
FORMAT OUT      FOUT2(8E10.3);
FORMAT OUT      HEADING1(//X55,"INPUT MATRIX A"//),
                FOUT1(X15,"ROW",I3/X15,"COLUMN"//(X15,5(I4,F15.8)));
LABEL           L1,L2,L3,L4,L5,L6,L7,L8,L9,N1,N2,N3,N4,N5,N6,N7,N8,N9;
                I = 1;
                J = 2;
                K = 3;
                L = 4;
                M = 5;
                N = 6;
                TEST = 0;
L1;             A[I,I]  =  A[I,I] + 4.32;
                A[J,J]  =  A[J,J] +12.00;
                A[K,I]  =  A[K,I] +43.20;
```

```
                A[K,K]  ←  A[K,K]+576.00;
                A[L,I]  ←  A[L,I] = 4.32;
                A[L,K]  ←  A[L,K] =43.20;
                A[L,L]  ←  A[L,L]  +4.32;
                A[M,J]  ←  A[M,J] =12.00;
                A[M,M]  ←  A[M,M] +12.00;
                A[N,I]  ←  A[N,I] +43.20;
                A[N,K]  ←  A[N,K]+288.00;
                A[N,L]  ←  A[N,L] =43.20;
                A[N,N]  ←  A[N,N]+576.00;
                I  ←  I +3;
                J  ←  J +3;
                K  ←  K +3;
                L  ←  L +3;
                M  ←  M +3;
                N  ←  N +3;
                IF TEST = 1  THEN GO TO N1;
                IF TEST = 2  THEN GO TO N2;
                IF TEST = 3  THEN GO TO N3;
                IF TEST = 4  THEN GO TO N4;
                IF TEST = 5  THEN GO TO N5;
COMMENT         TEST EQUALS 0;
                IF I ≤ 10  THEN GO TO L1;
                GO TO N6;
N1:             IF I≤ 25  THEN GO TO L1;
                GO TO N6;
N2:             IF I ≤ 40  THEN GO TO L1;
                GO TO N6;
N3:             IF I ≤ 55  THEN GO TO L1;
                GO TO N6;
N4:             IF I ≤ 70  THEN GO TO L1;
                GO TO N6;
N5:             IF I ≤ 85 THEN GO TO L1;
                GO TO L2;
N6:             I ← I +3;
                J ← J +3;
```

```
                    K ← K +3;
                    L ← L +3;
                    M ← M +3;
                    N ← N +3;
                    TEST ← TEST +1 ;
                    GO TO L1;
COMMENT             MATRIX ACROSS IS COMPLETE;
L2:                 I ← 1;
                    J ← 2;
                    K ← 3;
                    L ← 16;
                    M ← 17;
                    N ← 18;
                    TEST ← 0;
L3:                 A[I,I] ← A[I,I] + 12.00;
                    A[J,J] ← A[J,J] + 4.32;
                    A[K,J] ← A[K,J] + 43.20;
                    A[K,K] ← A[K,K] +576.00;
                    A[L,I] ← A[L,I] - 12.00;
                    A[L,L] ← A[L,L] + 12.00;
                    A[M,J] ← A[M,J] - 4.32;
                    A[M,K] ← A[M,K] - 43.20;
                    A[M,M] ← A[M,M] + 4.32;
                    A[N,J] ← A[N,J] + 43.20;
                    A[N,K] ← A[N,K] +288.00;
                    A[N,M] ← A[N,M] - 43.20;
                    A[N,N] ← A[N,N] +576.00;
                    I ← I+15;
                    J ← J+15;
                    K ← K+15;
                    L ← L+15;
                    M ← M+15;
                    N ← N+15;
                    IF TEST = 1 THEN GO TO L4;
                    IF TEST = 2 THEN GO TO L5;
                    IF TEST = 3 THEN GO TO L6;
```

```
                IF TEST = 4 THEN GO TO L7;
COMMENT         TEST = 0;
                IF I ≤ 61 THEN GO TO L3;
                GO TO L8;
L4:             IF I ≤ 64 THEN GO TO L3;
                GO TO L8;
L5:             IF I ≤ 67 THEN GO TO L3;
                GO TO L8;
L6:             IF I ≤ 70 THEN GO TO L3;
                GO TO L8;
L7:             IF I≤ 73 THEN GO TO L3;
                GO TO L9;
L8:             I ← I -72;
                J ← J -72;
                K ← K -72;
                L ← L -72;
                M ← M -72;
                N ← N -72;
                TEST ← TEST + 1;
                GO TO  L3;
COMMENT         ENTIRE LOWER HALF IS INPUT;
L9:             FOR I ← 1 STEP 1 UNTIL P-1 DO
                FOR J ← I +1 STEP 1 UNTIL P DO
                A[I,J] ← A[J,I];
                WRITE(PRINT,HEADING1);
                FOR I ← 1 STEP 1 UNTIL P DO
                WRITE(PRINT,FOUT1,MATRIN);
                FOR I ← 1 STEP 1 UNTIL P DO
                WRITE(PUNCH,FOUT2,LIST2);
        END
        END.
```

IV. PROGRAM DESCRIPTIONS

The following instructions for the use of the programs described here are correct as of the date of publication of this report. However, because card image tapes may be occasionally revised, it is recommended that the program tape or deck in the computer library be checked with the program listing shown in this report.

A. A Symmetric Matrix Inversion Routine Algol 60, MRS-095, B0005.

1. General Description

The inversion procedure originated from the Professional Services Group of the Burroughs Corporation. (Reference 8). The procedure uses a factorization technique to invert symmetric matrices whose leading sub-matrices are nonsingular, e. g. ,

$$[a_{11}] = 0, \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = 0, \ . \ . \ . \ , [A] = 0$$

If the matrix is known to be definite it can always be inverted by this method. The Procedure inverts the matrix and replaces the inverted matrix including the diagonal into the upper triangle of the original, with a savings of additional storage locations. The original diagonal is also preserved in a vector array and the remaining elements are left in their original positions in the lower triangular half upon exit from the procedure.

The particular Driver program listed here with the procedure punches and writes the inverted matrix in its entirety. The format declaration, HEAD2 should be printed if the unnumbered instructions between cards AW 502300 and AW 502400 are omitted. This Driver program was used after a Matrix Compile Program had punched the entire input matrix which was inverted on both symmetric and nonsymmetric inversion routines for comparison of results. Should a symmetric matrix be input from another source there is no need to input the entire array. If only the upper triangular half is input these same unnumbered instructions (between cards AW 502300 and AW 502400) can be utilized to complete the input. Even if the Procedure is followed directly by additional matrix operations, it is usually desirable to write (and often to punch cards) for the inverted matrix for an accuracy check as well as for future use.

2. Mathematical Theory

The Procedure utilizes a method of factoring attributed to Choleski and described in detail in Reference 1.

Briefly, a non-singular matrix, [A] may be factored into the product of an upper and lower triangular matrix

$$[A] = [U] \cdot [L]$$

when the matrix is symmetrical, it may be factored

$$[A] = [L]^T \cdot [D] \cdot [L]$$

where $[L]^T$ is the transpose of [L] and equal to the unit upper triangular matrix [U], and [D] is a diagonal matrix of the diagonal elements of [A]. Since the inverse of the transpose of a triangular matrix is equal to the transpose of the inverse from

$$[A]^{-1} = [L]^{T-1} \cdot [D] \quad [L]^{-1}$$

we can write

$$[A]^{-1} = [L]^{-1} \cdot [D] \cdot [L]^{T-1}$$

(This is valid from the theorem above and not from commutivity relations.) Therefore, the three inversions are carried out and then the inverted matrices are multiplied in reverse order to give the desired $[A]^{-1}$.

3. Accuracy and Machine Time

Several test cases were inverted by this method. A 50 × 50 matrix with elements within 2 orders of magnitude was inverted and the product of the original and inverted matrices yielded the unit matrix to four decimal places. A 90 × 90 matrix similarly well behaved yielded accuracy to only one decimal place. A 90 × 90 matrix with elements differing by 10^3 did not yield acceptable results and an iteration procedure using this inversion does not satisfy convergence criteria.

The approximate running time for the procedure is estimated as $.15\ N^3$ in Reference 8. Reading and writing are not included in this estimate.

DENVER, COLORADO, MAY 13, 1965

COPY OPTION = OMNI

```
          BEGIN                                                                  AW500100
COMMENT         MATRIX INVERSION USING LIBRARY PROCEDURE = A.WEST;               AW500200
FILE IN         CARD(2,10);                                                      AW500400
FILE OUT        PUNCH 0(2,10);                                                   AW500450
FILE OUT        LINE 4(2,15);                                                    AW500500
FORMAT IN       FMI2(I4);                                                        AW500600
FORMAT OUT      FMO2(8E10.3);                                                    AW501650
LABEL           L10,FINIS;                                                       AW500700
INTEGER         N,I,J;                                                           AW500800
REAL ARRAY      A[0:90,0:90],DIAGONAL[0:90];                                     AW500900
L10:            READ(CARD,FMI2,N) [FINIS];                                       AW501000
        BEGIN                                                                    AW501100
FORMAT IN       FMI1(8E10.3);                                                    AW501200
FORMAT OUT      HDG1(X15,"MATRIX INVERSION"//),                                  AW501300
                HDG2(X5,"UPPER TRIANGLE =INVERTED MAXTRIX, LOWER PART"           14
                    " IS ORIGINAL MATRIX"//),                                    AW501500
                FMO1(10(E12.3));                                                 AW501600
LABEL           FINIS,L10;                                                       AW501700
LIST            L1(FOR J+1 STEP 1 UNTIL N DO A[I,J]);                            AW501800
COMMENT         INVERSION PROCEDURE;                                             AW501900
```

```
PROCEDURE     INVPDS(N, A, DIAGONAL) ;                                           ISYM0130
VALUE         N ;                                                                ISYM0140
INTEGER       N ;                                                                ISYM0150
REAL ARRAY    A[0,0], DIAGONAL[0] ;                                              ISYM0160
        BEGIN                                                                    ISYM0170
```

```
INTEGER       I, J, K, I1, L ;                                          ISYM0180
REAL          DIAG, Q ;                                                 ISYM0190
REAL ARRAY    TEMP[0:N] ;                                               ISYM0200
LABEL         IN1, IN2, IN3 ;                                           ISYM0210
IN1:          FOR I ← N STEP -1 UNTIL 1 DO                              ISYM0260
        BEGIN                                                           ISYM0270
              DIAGONAL[I] ← A[I,I] ;                                    ISYM0280
              FOR K ← I+1 STEP 1 UNTIL N DO                             ISYM0290
              TEMP[K] ← A[I,K] × A[K,K] ;                               ISYM0300
              FOR J ← I STEP -1 UNTIL 1 DO                              ISYM0310
        BEGIN                                                           ISYM0320
              Q←0 ;                                                     ISYM0330
              FOR K ← I+1 STEP 1 UNTIL N DO Q ← A[J,K] × TEMP[K] + Q ;  ISYM0340
              IF I=J THEN A[J,I] ← DIAG ← A[J,I] - Q  ELSE              ISYM0350
                   A[J,I] ← (A[J,I]-Q)/DIAG                             ISYM0360
        END                                                             ISYM0370
        END ;                                                           ISYM0380
IN2:          FOR I ← N STEP -1 UNTIL 1 DO                              ISYM0400
        BEGIN                                                           ISYM0410
              I1 ← I+1 ;  A[I,I] ← 1.0 / A[I,I] ;                       ISYM0420
              FOR J ← N STEP -1 UNTIL I1 DO                             ISYM0430
        BEGIN                                                           ISYM0440
              Q←0 ;  L ← J-1 ;                                          ISYM0450
              FOR K ← I1 STEP 1 UNTIL L DO Q ← A[I,K] × A[K,J] + Q ;    ISYM0460
              A[I,J] ← -A[I,J] - Q                                      ISYM0470
        END                                                             ISYM0480
        END ;                                                           ISYM0490
IN3:          FOR I ← N STEP -1 UNTIL 1  DO                             ISYM0520
        BEGIN                                                           ISYM0530
              I1 ← I-1 ;  DIAG ← A[I,I] ;                               ISYM0540
              FOR K ← 1 STEP 1 UNTIL I1 DO                              ISYM0550
              TEMP[K] ← A[K,K] × A[K,I] ;                               ISYM0560
              FOR J ← N STEP -1 UNTIL I DO                              ISYM0570
        BEGIN                                                           ISYM0580
              Q←0 ;                                                     ISYM0590
              FOR K ← 1 STEP 1 UNTIL I1 DO Q ← A[K,J] × TEMP[K] + Q ;   ISYM0600
```

```
            A[I,J] ← IF I=J THEN A[I,J] + Q ELSE A[I,J] × DIAG + Q      ISYM0610
        END                                                             ISYM0620
        END                                                             ISYM0630
        END ;                                                           ISYM0640


            FOR I ←1, I+1 STEP 1 UNTIL N DO BEGIN                       AW502000
            READ(CARD,FMI1,L1);                                         AW502100
            END;                                                        AW502200
            INVPDS(N,A,DIAGONAL);                                       AW502300
            FOR I ← 1 STEP 1 UNTIL N-1 DO
            FOR J ← I+1 STEP 1 UNTIL N DO
            A[J,I] ← A[I,J];
            WRITE(LINE,HDG1);                                           AW502400
            FOR I ←1, I+1 STEP 1 UNTIL N DO BEGIN                       AW502600
            WRITE(LINE,FMO1,L1);                                        AW502700
            END;                                                        AW502800
            FOR I ← 1, I+1 STEP 1 UNTIL N DO BEGIN
            WRITE(PUNCH, FMO2, L1);
            END;
        END;                                                            AW502900
FINIS:  END.                                                            AW503000
```

4. Input Format

If a matrix is to be inverted by this Procedure with the Driver program listed here, the input formats should be as follows.

First Card — Columns 1 - 4

An integer, N, indicating the order of the square matrix, right justified in column 4.

Example

Column	1 - 4
Data	16

Second Card — Columns 1 - 80 contain the elements of the first row written in floating point notation in 8E10. 3 format.

Example $\pm$ 0. xxx@$\pm$ee

where "ee" indicates the power of 10 to which the number is to be raised after expressing it as a decimal whose first digit to the right of the decimal point is non-zero. Eight elements can be punched across the 80 column card. No spaces are permitted between elements. An entire blank field (all 10 columns) is permitted for inputting zero elements. Succeeding cards are used until the entire first row is input.

New Card — Each new row is begun on a new card.

5. Alternate Input for Sparse Matrices

If a machine compile program is not used, and if the matrix is sparse, it will be more convenient to input only those elements which are non-zero. The program listed here can be altered slightly to accept this type input.

Omit cards AW502000 - AW502200

In their place insert

```
          BEGIN
LIST            LL1(A[n, n], A[n, n], A[n, n], ... A[n, n]);
                READ (CARD, FMI1, LL1);
          END;
```

where each A[n, n] corresponds to the appropriately positioned data element.

Example:

$$\begin{bmatrix} 1 & 1 & 2 \\ 0 & 10 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

```
          BEGIN
LIST            LL1(A[1, 1], A[1, 2], A[1, 3], A[2, 2], A[3, 3]);
                READ (CARD, FMI1, LL1);
          END;
```

with the following data card, beginning in column 1

```
1          11          21          31          41
+0.100@+01+0.100@+01+0.200@+01+0.100@+02+0.500@01
```

If more than 80 elements are to be input the LIST and READ statements should be segmented into groups of 80 and should be enclosed in BEGIN and END statements.

B. A Program to Determine the Eigenvalues of a Real Symmetric Matrix Using Givens' Method, MRS-028(Reference 9).

This program EIGEN, is given in its entirety in Reference 9 together with a full mathematical discourse, and will not be reproduced here. The program was checked alone and with additional subroutines for determining the associated eigenvectors. This procedure solves for the eigenvalues only. One format must be changed to permit input of large matrices (the test case is for n = 8). Card number TEST0014 now reads

FØRMAT IN FIN1 (I1);

and should be changed to read

FØRMAT IN FIN1 (I3).

Another card which may have to be changed, depending upon the input information, is card number TEST0030. It now calls for inputs in the form F6.1

xxxx.x .

For numbers much less than 1 this will not be a satisfactory format, and should be changed accordingly. Test cases were run with format

8F9.4 , $\overline{x}$xxx.xxxx .

Briefly, the program begins by reducing the input matrix A to tridiagonal form. The leading principle minors of the reduced matrix form a STURM sequence which is used in a bisection process which is terminated when λ is isolated in a sub-interval [a, b] such that $[a-b] < \epsilon$. The epsilon is computed by the program as a function of the magnitude of lambda; $\epsilon = 10^{p-11}$ where p is the number of digits occurring to the left of the decimal point of λ .

The procedure prints out the full set of eigenvalues and the epsilon computed for each.

The output from this program was used to calculate the eigenvectors of the same system. This was accomplished by a driver program which called for the procedure SØLVE which solves a set of n simultaneous non-homogeneous equations. This method was used to compare accuracy with the translated program TEEV which solves for both the eigenvalues and the vectors and is described in the next section.

1. The Set of Homogeneous Equations

$$([A] - \lambda_i \ [I]) \ \{X\} = 0 \qquad (1)$$

where λ i is any one of the eigenvalues calculated by EIGEN may be solved as follows.

allowing Xn = 1 (since the solution of the homogeneous set of equations can be obtained only to within some multiplicative constant) the set of equations (1) can be written for each lambda

$$
\begin{array}{llll}
a_{11} - \lambda i & a_{12} & a_{13} \ldots a_{1\,n-1} & = -a_{1n} \\
a_{21} & a_{22} - \lambda i & a_{23} \ldots a_{2\,n-1} & = -a_{2n} \\
\cdot & \cdot & \cdot & = \cdot \\
\cdot & \cdot & \cdot & = \cdot \\
\cdot & \cdot & \cdot & = \cdot \\
a_{n-1,\,1} & a_{n-1,\,2} & \cdot \quad a_{n-1\,n-1} - \lambda_i & = -a_{n-1\,n}
\end{array}
$$

This set of equations is solved separately for each λi for which the corresponding vector is desired.

2. Accuracy

The accuracy for this program was compared with the following program (TEEV) and the results in 2 cases are given at the end of the following section, together with the "exact" solutions for each.

C. Eigenvalue - Eigenvector Program, TEEV, from SHARE subroutine HOW, A Fortran Program (Reference 10).

A large part of the effort expended on Project 618 involved the translation of this SHARE program from Fortran to Algol. The program is mathematically very similar to the procedure EIGEN described in the previous section. The accuracy is somewhat better due to a more sophisticated sequence for isolating the eigenvalues between smaller and smaller bounds and the program goes on to solve for the eigenvectors of the diagonalized matrix, which is much more efficient than the simultaneous equation solution using the original matrix, the procedure for which is outlined in the preceding section. Previously this was the only method available for solution of the modal vectors.

The problems encountered in translating this group of subroutines into Algol are not properly a subject for this report. One particular problem; however, which was overcome only by some rather unorthodox input instructions, is described here mainly as explanation for the input and secondly as general information regarding Fortran and Algol monitoring systems.

The Fortran monitoring system allows a subroutine to define its parameters independently of its calling sequence. That is, a non-arrayed subroutine parameter may be called from an arrayed parameter, taking the current value for the subscript, or, as in the case of the input matrix to this program, a two-dimensional matrix array may be treated as a one-dimensional parameter in a subroutine. The Algol monitor objects to this sort of thing quite vigorously - it refuses to compile until parameters agree as to type and number of dimensions. Therefore it was necessary to go through the program and redefine parameters where necessary before calling a procedure so that the properly positioned array parameter was called in a manner compatible with Algol compilation. Therefore, the $n \times n$ input matrix [S] is read in as a vector {S} of length n^2. Since this program is valid for symmetrical matrices only it is not important that the input be made by rows or columns, providing a consistant method is employed for numbering the elements 1 through n^2.

1. Input

If the procedure TEEV is used with the driver program shown here, the input should be as follows:

First Card (Format 3I4)

Input for N, M, MAXN where

N - order of the input matrix [S]
Range $1 \leq N \leq 175$

M - absolute value of M where $0 \leq M \leq N$ indicates the number of eigenvectors to be calculated. The ordering of the eigenroots, to which the calculated eigenvectors will correspond, is determined by the sign of M as follows:

$M > 0$, $M = +0$ } Eigenroots arranged in descending absolute value

$M < 0$, $M = -0$ } Eigenroots arranged in ascending absolute value

MAXN - the maximum order N may obtain, i. e., the value in the array statement in the main program. Unless this group of subroutines is called from another program, MAXN = N.

Example: For a 50 × 50 matrix whose eigenvectors corresponding to the 5 lowest modes of vibrations are desired, the first card would read

```
COLUMN  1 2 3 4 5 6 7 8 9 10 11 12
DATA        5 0     - 5       5  0
```

Please note that these are integer numbers written without decimal points and are right-justified in columns 4, 8 and 12.

Second and Succeeding Cards (Format 6E12. 4)

Input for the vector {S} of length n^2

Six elements are entered on each card until the entire array is read into the computer. The entries are made either by row or by column of the symmetric matrix [S].

An E12. 4 format indicates the following:

±0. xxxx@±ee

where ee indicates the power of ten to which the number must be raised to allow the first non-zero digit to appear immediately to the right of the decimal point. The elements will be right-justified in columns 12, 24, 48 and 72. The first number would therefore start in column 2.

Example: Input the number 3, 285. 0

```
COLUMN  1 2 3 4 5 6 7 8 9 10 11 12
DATA      + 0 . 3 2 8 5 @ +  0  4
```

2. Machine Time and Accuracy

Although this SHARE program has been documented at the National Bureau of Standards SHARE library to have been used successfully on IBM equipment for matrices as large as n = 175, the largest problem run here with good accuracy (on the B5500) with the translated program was a 75 × 75 well behaved matrix. Eigenvalues for a less well behaved 90 × 90 matrix did not yield satisfactory results. Machine time was not

the problem it was anticipated to be. The full set of eigenvalues and eigenvectors for the 75 × 75 matrix were run in less than 30 minutes (clock time) which is approximately double the actual processing time.

A comparison of the eigenvalues of an 8 × 8 matrix from the procedure EIGEN and this procedure TEEV showed excellent agreement with the exact solutions and with each other. As the order of the matrix increased, the translated program TEEV produced more accurate results than the procedure EIGEN. For eigenvalues only, the procedure EIGEN uses less machine time. For a matrix of order 24 the EIGEN procedure took 24 seconds running time and the TEEV procedure took 36 seconds running time.

D. Inverse of a Non-Symmetric Matrix

After this study was initiated a program for finding the inverse of a non-symmetric matrix was checked out by Computer Center personnel. This program, B0004 "Inverse of a Matrix" Technical Bulletin MRS-093/R is in the Computer Library with a sample driver program and is ready for production runs.

Another program, SHARE program INVRS written in Fortran IV has been requested from IBM in New York and will be translated into Algol when it arrives. It is reputed to solve for the inverse of general matrices up to order 2000. No program listing or mathematical description was given but the program will be reviewed and, if feasible, processed here as soon as it is available.

DENVER, COLORADO, MAY 27, 1965

COPY OPTION - OMNI

```
COMMENT  TEEV TRANSLATED EIGENVALUE EIGENVECTOR PROGRAM   A. WEST;
BEGIN                                                                  00001000
FILE IN CARD 0(2,10);     FILE OUT  LINE 4(2,15);                      00002000
FILE OUT PUNCH 0(2,10);                                                00003000
BOOLEAN ARRAY  SENSL[0:4];                                             00004000
REAL  XPR;                                                             00005000
INTEGER  QQ;                                                           00006000
LABEL FINIS;                                                           00007000
PROCEDURE ERROR(N); VALUE N; INTEGER N; BEGIN                          00008000
  FORMAT F(////////"STOP / PAUSE  NO. ", I5);                          00009000
  WRITE (LINE,  F, N); GO TO FINIS END;                                00010000
REAL PROCEDURE INT(ARG1); VALUE ARG1; REAL ARG1;                       00011000
    BEGIN INT←(SIGN(ARG1)×ENTIER(ABS(ARG1))) END;                      00012000
REAL PROCEDURE MAX(ARG1,ARG2); VALUE ARG1,ARG2; REAL ARG1,ARG2;        00013000
  BEGIN MAX←(IF ARG1≥ARG2 THEN ARG1 ELSE ARG2) END;                    00014000
REAL PROCEDURE MIN(ARG1,ARG2); VALUE ARG1,ARG2; REAL ARG1,ARG2;        00015000
  BEGIN MIN←(IF ARG1≤ARG2 THEN ARG1 ELSE ARG2) END;                    00016000
PROCEDURE TRIDIQ(LPQ,NMQ,R,A,B,W,Q);
       VALUE LPQ,NMQ;
       INTEGER LPQ,NMQ;
       REAL ARRAY R[0], A[0],B[0],W[0],Q[0];
       FORWARD;
PROCEDURE EIGVALQ(LPQ,NMQ,M,E,A,B,F,W);
       VALUE LPQ,NMQ;
       INTEGER LPQ,NMQ,M;
       REAL ARRAY E[0],A[0],B[0],F[0],W[0];
       FORWARD;
PROCEDURE EIGVECQ(LPQ,NMQ,R,A,B,E,V,P,Q);
```

```
        VALUE LPQ,NMQ,E;
        INTEGER LPQ,NMQ;
        REAL E;
        REAL ARRAY R[0],A[0],B[0],V[0],P[0],Q[0];
        FORWARD;
COMMENT ************************** HOW ****************;                    00017000
PROCEDURE HOWQ(LPQ,NMQ,M,R,E,V,A,B,W1Q,W2Q);                              00018000
        INTEGER LPQ,NMQ,M;                                                00019000
        REAL ARRAY  R[0],E[0],V[0],A[0],B[0],W1Q[0],                      00020000
          W2Q[0];                                                         00021000
BEGIN                                                                     00022000
OWN INTEGER K, J, I, NM1Q, JJQ, LP2Q,DX1;                                 00023000
        OWN REAL  TE;                                                     00023500
COMMENT  THE FOLLOWING SUBROUTINES ARE REQUIRED:                          00024000
          TRIDI, EIGVAL, EIGVEC;                                          00025000
LABEL DUMMY,L4,L5,L9,L14,L20;                                             00026000
FORMAT
   HEAD3(//X10,"EIGENVECTORS"//);                                         00328700
FORMAT  FL6(6E12.4);
LIST LIST4(FOR DX1 ← 1 STEP 1 UNTIL K   DO V[DX1]);                       00332000
          IF (XPR ← LPQ=1)>0 THEN GO TO L4;                               00027000
          IF XPR=0 THEN GO TO L14 ELSE GO TO DUMMY;                       00028000
          COMMENT                                                         00029000
    TRI-DIAGONALIZE MATRIX;                                               00030000
L4:       TRIDIQ(LPQ,NMQ,R,A,B,W1Q,W2Q);                                  00031000
          COMMENT                                                         00032000
    FIND EIGEN VALUES;                                                    00033000
          EIGVALQ(LPQ,NMQ,M,E,A,B,W1Q,W2Q);                               00034000
          IF M=0 THEN GO TO L9 ELSE GO TO L5;                             00035000
          COMMENT                                                         00036000
    FIND EIGEN VECTORS;                                                   00037000
L5:       K ← ABS(M);                                                     00038000
          J ← 1;                                                          00039000
          FOR I ← 1, I+1 STEP 1 UNTIL K DO BEGIN                          00040000
               TE ← E[I];                                                 00040500
            EIGVECQ(LPQ,NMQ,R,A,B,TE,  V,   W1Q,W2Q);                     00041000
```

```
    WRITE (LINE,HEAD3);                                                    00338500
WRITE (LINE,FL6,LIST4);
            J ← J+NMQ  END;                                                00042000
          COMMENT                                                          00043000
    RESTORE INPUT MATRIX;                                                  00044000
L9:       NM1Q ← NMQ+1;                                                    00045000
          JJQ ← NM1Q;                                                      00046000
          LP2Q ← LPQ×NMQ;                                                  00047000
          FOR I ← 2, I+NM1Q STEP NM1Q UNTIL LP2Q DO BEGIN                  00048000
            K ← I;                                                         00049000
            FOR J ← JJQ, J+NMQ STEP NMQ UNTIL LP2Q DO BEGIN                00050000
              R[K] ← R[J];                                                 00051000
              K ← K+1  END;                                                00052000
            JJQ ← JJQ+NM1Q  END;                                           00053000
          GO TO DUMMY;                                                     00054000
          COMMENT                                                          00055000
    SOLUTION FOR ORDER 1;                                                  00056000
L14:      E[1] ← R[1];                                                     00057000
          V[1] ← 1;                                                        00058000
          A[1] ← R[1];                                                     00059000
          B[1] ← 0;                                                        00060000
L20:      GO TO DUMMY;                                                     00061000
DUMMY:    END;                                                             00062000
                                                                           00063000
COMMENT ***************************  TRIDI  ****************;             00064000
PROCEDURE TRIDIQ(LPQ,NMQ,R,A,B,W,Q);                                       00065000
        VALUE LPQ,NMQ;                                                     00066000
        INTEGER LPQ,NMQ;                                                   00067000
        REAL ARRAY  R[0],A[0],B[0],W[0],Q[0];                              00068000
BEGIN                                                                      00069000
OWN INTEGER LP1Q, LP2Q, LPPQ, NM1Q, L, I, KKQ, K, KLQ, KUQ, KJQ,           00070000
        J, JJQ, LLQ;                                                       00071000
OWN REAL SUMQ, S, X;                                                       00072000
LABEL DUMMY,L36,L65,L99;                                                   00073000
          LP1Q ← LPQ-1;                                                    00074000
          LP2Q ← LP1Q×NMQ+LPQ;                                             00075000
```

```
        LPPQ ← LP2Q-NMQ;                                                    00076000
        NM1Q ← NMQ+1;                                                       00077000
        COMMENT                                                             00078000
  STORE ORIGINAL DIAGONAL;                                                  00079000
        L ← 0;                                                              00080000
        FOR I ← 1, I+NM1Q STEP NM1Q UNTIL LP2Q DO BEGIN                     00081000
          L ← L+1;                                                          00082000
          A[L] ← R[I]  END;                                                 00083000
        B[1] ← 0;                                                           00084000
        IF (XPR ← LPQ-2)=0 THEN GO TO L65;                                  00085000
        IF XPR<0 THEN GO TO DUMMY;                                          00086000
        KKQ ← 0;                                                            00087000
        FOR K ← 2, K+1 STEP 1 UNTIL LP1Q DO BEGIN                           00088000
          KLQ ← KKQ+K;                                                      00089000
          KUQ ← KKQ+LPQ;                                                    00090000
          KJQ ← K+1;                                                        00091000
          COMMENT                                                           00092000
  CALCULATE AND STORE MODIFIED COLUMN MATRIX W;                             00093000
          SUMQ ← 0;                                                         00094000
          FOR J ← KLQ, J+1 STEP 1 UNTIL KUQ DO BEGIN                        00095000
            SUMQ ← SUMQ+R[J]↑2  END;                                        00096000
          S ← SQRT(SUMQ);                                                   00097000
          B[K] ← (ABS(S)×SIGN(-R[KLQ]));                                    00098000
          S ← 1/S;                                                          00099000
          W[K] ← SQRT(ABS(R[KLQ])×S+1);                                     00100000
          X ← (ABS(S/W[K])×SIGN(R[KLQ]));                                   00101000
          R[KLQ] ← W[K];                                                    00102000
          FOR I ← KJQ, I+1 STEP 1 UNTIL LPQ DO BEGIN                        00103000
            JJQ ← I+KKQ;                                                    00104000
            W[I] ← X×R[JJQ];                                                00105000
            R[JJQ] ← W[I]  END;                                             00106000
          COMMENT                                                           00107000
  CALCULATE NEW R MATRIX WITH ROW K-1 NOW HAVING ZEROS OFF 2ND DIAGONA      00108000
          L;                                                                00109000
          FOR J ← K, J+1 STEP 1 UNTIL LPQ DO BEGIN                          00110000
            JJQ ← J+1;                                                      00111000
```

```
                Q[J] ← 0;                                                00112000
                L ← KKQ+J;                                               00113000
                FOR I ← K, I+1 STEP 1 UNTIL J DO BEGIN                   00114000
                  L ← L+NMQ;                                             00115000
                  Q[J] ← Q[J]+R[L]×W[I]  END;                            00116000
                IF JJQ>LPQ THEN GO TO L36;                               00117000
                FOR I ← JJQ, I+1 STEP 1 UNTIL LPQ DO BEGIN               00118000
                  L ← L+1;                                               00119000
                  Q[J] ← Q[J]+R[L]×W[I]  END;                            00120000
                END;                                                     00121000
L36:          X ← 0;                                                     00122000
              FOR J ← K, J+1 STEP 1 UNTIL LPQ DO BEGIN                   00123000
                X ← X+W[J]×Q[J]  END;                                    00124000
              X ← ,5×X;                                                  00125000
              FOR I ← K, I+1 STEP 1 UNTIL LPQ DO BEGIN                   00126000
                Q[I] ← X×W[I]-Q[I]  END;                                 00127000
              LLQ ← KKQ;                                                 00128000
              KKQ ← KKQ+NMQ;                                             00129000
              FOR I ← K, I+1 STEP 1 UNTIL LPQ DO BEGIN                   00130000
                LLQ ← LLQ+NMQ;                                           00131000
                FOR J ← I, J+1 STEP 1 UNTIL LPQ DO BEGIN                 00132000
                  L ← LLQ+J;                                             00133000
                  R[L] ← R[L]+Q[I]×W[J]+Q[J]×W[I]  END;                  00134000
                END;                                                     00135000
              END;                                                       00136000
            COMMENT                                                      00137000
      SORT OUTPUT;                                                       00138000
            L ← 1;                                                       00139000
            FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                     00140000
              X ← A[I];                                                  00141000
              A[I] ← R[L];                                               00142000
              R[L] ← X;                                                  00143000
              L ← L+NM1Q  END;                                           00144000
L65:        B[LPQ] ← R[LPPQ];                                            00145000
L99:        GO TO DUMMY;                                                 00146000
DUMMY:      END;                                                         00147000
```

```
                                                                    00148000
COMMENT ***************************  EIGVAL  ****************;      00149000
PROCEDURE EIGVALQ(LPQ,NMQ,M,E,A,B,F,W);                             00150000
        VALUE LPQ,NMQ;                                              00151000
        INTEGER LPQ,NMQ,M;                                          00152000
        REAL ARRAY  E[0],A[0],B[0],F[0],W[0];                       00153000
BEGIN                                                               00154000
REAL ARRAY  ARRAY1[0:1];                                            00155000
  DEFINE  S1Q     =ARRAY1[1]#;                                      00156000
  DEFINE  IS1Q    =ARRAY1[1]#;                                      00157000
REAL ARRAY  ARRAY2[0:1];                                            00158000
  DEFINE  IS2Q    =ARRAY2[1]#;                                      00159000
  DEFINE  S2Q     =ARRAY2[1]#;                                      00160000
OWN INTEGER I, K, N, J;                                             00161000
OWN REAL BDQ, X;                                                    00162000
LABEL DUMMY,L8,L104,L105,L112,L113,L114,L115,L117,L120,L20,L50,L65,  00163000
      L70,L80;                                                      00164000
        COMMENT                                                     00165000
    FIND UPPER AND LOWER BOUNDS AND NORMALIZE INPUT;                00166000
        BDQ ← ABS(A[1]);                                            00167000
        FOR I ← 2, I+1 STEP 1 UNTIL LPQ DO BEGIN                    00168000
          BDQ ← MAX(BDQ,ABS(A[I])+B[I]*2)  END;                     00169000
        BDQ ← BDQ+1;                                                00170000
        FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                    00171000
          A[I] ← A[I]/BDQ;                                          00172000
          B[I] ← B[I]/BDQ;                                          00173000
          W[I] ← 1;                                                 00174000
          E[I] ← -1  END;                                           00175000
        FOR K ← 1, K+1 STEP 1 UNTIL LPQ DO BEGIN                    00176000
L8:       IF (W[K]-E[K])/MAX(MAX(ABS(W[K]),ABS(E[K])),1             00177000
            @-9)≤1@-7 THEN GO TO L50;                               00178000
          X ← (W[K]+E[K])×,5;                                       00179000
          COMMENT                                                   00180000
    FIND NUMBER OF EIGEN VALUES ,N, GREATER THAN OR EQUAL TO X;     00181000
          IS2Q ← INT(1);                                            00182000
          F[1] ← A[1]-X;                                            00183000
```

```
            IF F[1]≥0 THEN GO TO L104;                                  00184000
            IS1Q ← INT(-1);                                             00185000
            N ← 0;                                                      00186000
            GO TO L105;                                                 00187000
L104:       IS1Q ← INT(1);                                              00188000
            N ← 1;                                                      00189000
L105:       FOR I ← 2, I+1 STEP 1 UNTIL LPQ DO BEGIN                    00190000
              IF B[I]=0 THEN GO TO L113;                                00191000
              IF B[I-1]=0 THEN GO TO L114;                              00192000
              IF ABS(F[I-1])+ABS(F[I-2])≥1@-15 THEN GO TO L112;         00193000
              F[I-1] ← F[I-1]×1@15;                                     00194000
              F[I-2] ← F[I-2]×1@15;                                     00195000
L112:         F[I] ← (A[I]-X)×F[I-1]-B[I]*2×F[I-2];                     00196000
              GO TO L115;                                               00197000
L113:         F[I] ← (A[I]-X)×(ABS(1)×SIGN(S1Q));                       00198000
              GO TO L115;                                               00199000
L114:         F[I] ← (A[I]-X)×F[I-1]-(ABS(B[I]*2)×SIGN(S2Q)             00200000
                );                                                      00201000
L115:         S2Q ← S1Q;                                                00202000
              IF F[I]=0 THEN GO TO L117;                                00203000
              S1Q ← (ABS(S1Q)×SIGN(F[I]));                              00204000
              IF IS2Q+IS1Q=0 THEN GO TO L120;                           00205000
L117:         N ← N+1;                                                  00206000
L120:         END;                                                      00207000
            COMMENT                                                     00208000
        TRAP EIGEN VALUES IN SMALLER AND SMALLER BOUNDS;                00209000
            N ← LPQ-N;                                                  00210000
            IF N<K THEN GO TO L20;                                      00211000
            FOR J ← K, J+1 STEP 1 UNTIL N DO BEGIN                      00212000
              W[J] ← X  END;                                            00213000
L20:        N ← N+1;                                                    00214000
            IF LPQ<N THEN GO TO L8;                                     00215000
            FOR J ← N, J+1 STEP 1 UNTIL LPQ DO BEGIN                    00216000
              IF X≤E[J] THEN GO TO L8;                                  00217000
              E[J] ← X  END;                                            00218000
            GO TO L8;                                                   00219000
```

```
L50:        END;                                                          00220000
          COMMENT                                                         00221000
     RESTORE INPUT AND ORDER EIGEN VALUES;                                00222000
          FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                        00223000
            A[I] ← A[I]×BDQ;                                              00224000
            B[I] ← B[I]×BDQ;                                              00225000
            F[I] ← (W[I]+E[I])×BDQ×.5  END;                               00226000
          J ← LPQ;                                                        00227000
          K ← 1;                                                          00228000
          FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                        00229000
            IF ABS(F[K])>ABS(F[J]) THEN GO TO L65;                        00230000
            E[I] ← F[J];                                                  00231000
            J ← J-1;                                                      00232000
            GO TO L70;                                                    00233000
L65:        E[I] ← F[K];                                                  00234000
            K ← K+1;                                                      00235000
L70:        END;                                                          00236000
          IF (ABS(1)×SIGN(M))≥0 THEN GO TO L80;                           00237000
          FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                        00238000
            F[I] ← E[I]  END;                                             00239000
          J ← LPQ;                                                        00240000
          FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                        00241000
            E[I] ← F[J];                                                  00242000
            J ← J-1  END;                                                 00243000
L80:      GO TO DUMMY;                                                    00244000
DUMMY:    END;                                                            00245000
                                                                          00246000
COMMENT ***************************  EIGVEC  ****************;           00247000
PROCEDURE EIGVECQ(LPQ,NMQ,R,A,B,E,V,P,Q);                                 00248000
        VALUE LPQ,NMQ,E;                                                  00249000
        INTEGER LPQ,NMQ;                                                  00250000
        REAL E;                                                           00251000
        REAL ARRAY  R[0],A[0],B[0],V[0],P[0],Q[0];                        00252000
BEGIN                                                                     00253000
OWN INTEGER LP1Q, I, J, K, L;                                             00254000
OWN REAL X, Y, Z;                                                         00255000
```

```
LABEL DUMMY,L6,L8,L10,L22,L25,L28,L30,L32,L42;                    00256000
        COMMENT                                                   00257000
    SET UP SIMULTANEOUS EQUATIONS FOR EIGEN VECTOR WITH EIGEN VALUE E; 00258000
        X ← A[1]-E;                                               00259000
        Y ← B[2];                                                 00260000
        LP1Q ← LPQ-1;                                             00261000
        FOR I ← 1, I+1 STEP 1 UNTIL LP1Q DO BEGIN                 00262000
          IF (XPR ← ABS(X)-ABS(B[I+1]))>0 THEN GO TO L8;          00263000
          IF XPR=0 THEN GO TO L6;                                 00264000
          P[I] ← B[I+1];                                          00265000
          Q[I] ← A[I+1]-E;                                        00266000
          V[I] ← B[I+2];                                          00267000
          Z ← -X/P[I];                                            00268000
          X ← Z×Q[I]+Y;                                           00269000
          IF LP1Q=I THEN GO TO L10;                               00270000
          Y ← Z×V[I];                                             00271000
          GO TO L10;                                              00272000
L6:       IF X≠0 THEN GO TO L8;                                   00273000
          X ← 1@-10;                                              00274000
L8:       P[I] ← X;                                               00275000
          Q[I] ← Y;                                               00276000
          V[I] ← 0;                                               00277000
          X ← A[I+1]-(B[I+1]/X×Y+E);                              00278000
          Y ← B[I+2];                                             00279000
L10:      END;                                                    00280000
        COMMENT                                                   00281000
    SOLVE SIMULTANEOUS EQUATIONS FOR EIGEN VECTOR OF TRI-DIAGONAL MATRIX00282000
          ;                                                       00283000
        IF X=0 THEN GO TO L28;                                    00284000
        V[LPQ] ← 1/X;                                             00285000
L22:    I ← LP1Q;                                                 00286000
        V[I] ← (1-Q[I]×V[LPQ])/P[I];                              00287000
        X ← V[LPQ]*2+V[I]*2;                                      00288000
L25:    I ← I-1;                                                  00289000
        IF I=0 THEN GO TO L30;                                    00290000
        V[I] ← (1-(Q[I]×V[I+1]+V[I]×V[I+2]))/P[                   00291000
```

```
                I];                                                    00292000
              X ← X+V[I]*2;                                            00293000
              GO TO L25;                                               00294000
L28:          V[LPQ] ← 1@10;                                           00295000
              GO TO L22;                                               00296000
L30:          X ← SQRT(X);                                             00297000
              FOR I ← 1, I+1 STEP 1 UNTIL LPQ DO BEGIN                 00298000
                V[I] ← V[I]/X  END;                                    00299000
              COMMENT                                                  00300000
        TRANSFORM EIGEN VECTOR TO SOLUTION OF ORIGINAL MATRIX;         00301000
              J ← LP1Q×NMQ-NMQ;                                        00302000
              K ← LPQ;                                                 00303000
              GO TO L42;                                               00304000
L32:          K ← K-1;                                                 00305000
              J ← J-NMQ;                                               00306000
              Y ← 0;                                                   00307000
              FOR I ← K, I+1 STEP 1 UNTIL LPQ DO BEGIN                 00308000
                L ← J+I;                                               00309000
                Y ← Y+V[I]×R[L]  END;                                  00310000
              FOR I ← K, I+1 STEP 1 UNTIL LPQ DO BEGIN                 00311000
                L ← J+I;                                               00312000
                V[I] ← V[I]-Y×R[L]  END;                               00313000
L42:          IF J≠0 THEN GO TO L32;                                   00314000
              GO TO DUMMY;                                             00315000
DUMMY:        END;                                                     00316000
                                                                       00317000
COMMENT ***************************  MAINPRO  ****************;       00318000
PROCEDURE MAINPRO;                                                     00319000
BEGIN                                                                  00320000
OWN REAL ARRAY   S[0:64], R[0:64], V[0:64], B[0:64],                   00321000
        W1Q[0:64], W2Q[0:64], A[0:64];                                 00322000
INTEGER  DX1;                                                          00323000
OWN INTEGER N, M, NNQ, MAXNQ;                                          00324000
COMMENT  THE FOLLOWING SUBROUTINES ARE REQUIRED:                       00325000
              HOW;                                                     00326000
FORMAT IN  FL1(6E12.4),                                                00327000
```

```
        FL2(I4,I4,I4);                                                    00328000
FORMAT       FL3(3E12.4),                                                 0032710
        HEAD1 (X10, "INPUT MATRIX"//),                                    00328500
   HEAD2(//X10,"EIGENVALUES"//));
LIST LIST1(N,M,MAXNQ),                                                    00329000
     LIST2(FOR DX1 ← 1 STEP 1 UNTIL NNQ DO S[DX1]),                       00330000
     LIST3(FOR DX1 ← 1 STEP 1 UNTIL N DO R[DX1]);                         00331000
          READ(CARD,FL2,LIST1)[FINIS];                                    00333000
          NNQ ← NxN;                                                      00334000
          READ(CARD,FL1,LIST2)[FINIS];                                    00335000
          HOWQ(N,MAXNQ,M,S,R,V,A,B,W1Q,W2Q);                              00336000
WRITE(LINE[PAGE]);
     WRITE(LINE,HEAD1);                                                    0336500
          WRITE(LINE,FL3,LIST2);                                          00337000
     WRITE(LINE,HEAD2);                                                   00337500
          WRITE(LINE,FL3,LIST3);                                          00338000
          END;                                                            00340000
                                                                          00341000
COMMENT ***************************  OUTER BLOCK  ************;         00342000
  XPR←QQ←0;                                                               00343000
            SENSL[1]←FALSE;                                               00344000
            SENSL[2]←FALSE;                                               00345000
            SENSL[3]←FALSE;                                               00346000
            SENSL[4]←FALSE;                                               00347000
MAINPRO; FINIS;                                                           00348000
END OF OUTER BLK.                                                         00349000
```

V. ADDITIONAL REMARKS AND CONCLUSIONS

Finally, it should be mentioned that any program which solves systems of non-homogeneous equations, especially if set up to work with multiple right hand sides, can be utilized in the solution of a matrix inversion. This can be demonstrated:

Given $[A] \cdot \{X\} = \{C\}$

where $[A]$ is the coefficient matrix of the unknown column matrix $\{X\}$, and $\{C\}$ is also a column matrix, then

$$\{X\} = [A]^{-1} \cdot \{C\}$$

Now, if $\{C\}$ is input, column by column, as the Identity Matrix (zeros on all but the main diagonal of ones)

$$[A] \cdot \{X\} = [I_j]$$

then $$\{X\} = [A]^{-1} \cdot \{I_j\} = [A]^{-1}$$

If $\{C\}$ is input as the individual columns of the Identity Matrix, $[I]$, then the n solutions for $\{X\}$ will be the n columns of the inverted matrix, $[A]^{-1}$.

This procedure for solving for matrix inversion is not as inefficient as it may first appear to be. The reduction of the coefficient matrix $[A]$ is the bulk of the computation, and solutions for the additional columns of the identity matrix can usually be done very rapidly. A Fortran-FAP program from the National Bureau of Standards (Boulder) and a Fortran-Machine Language program from the Martin Company for solving very large systems of simultaneous equations (and for inverting very large matrices) are referenced in the Appendix.

Although we appear to have the tools for calculating inversions of very large matrices and for finding the eigenvalues and vectors for matrices as large as $n \approx 100$, we cannot be assured of satisfactory solutions for these problems. The mathematical methods utilized in our programs are standard procedures for accomplishing these operations. Unless, however, we work with extremely well behaved and well conditioned (single element dominance in each row) our capability is considerably less than this. Double precision arithmetic would undoubtedly be of great value and the possibility of using these programs with double precision routines should be investigated.

We will probably encounter machine time problems by doing this, but it may be a necessary price. Additional auxiliary equipment, such as tape units, may be the only practical answer for extending solutions of eigenvalue problems to larger sized matrices. This is an expensive suggestion but the price and the inconvenience of using outside contracts for these solutions is far from inexpensive.

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DENVER, COLORADO, MAY 11, 1965

COPY OPTION - OMNI

```
COMMENT     MATRIX ITERATION SAMPLE PROGRAM    A. WEST;
            BEGIN
FILE IN         CARD (2,10);
FILE OUT        LINE 4(2,15);
FORMAT IN       FIN (4F12.3);
FORMAT OUT      FOT (4F12.3);
INTEGER         I,J,K;
FORMAT OUT      FOT2(//);
ARRAY           A[0:4,0:4],B[0:4,0:4],D[0:4,0:4];
LIST            L1(FOR J ←1 STEP 1 UNTIL 4 DO A[I,J]),
                L2(FOR J ←1 STEP 1 UNTIL 4 DO B[I,J]),
                L3(FOR J ←1 STEP 1 UNTIL 4 DO D[I,J]);
PROCEDURE       MATRIT(N,A,B,EPSIL);
VALUE           N;
INTEGER         N;
ARRAY           A[0,0], B[0,0];
REAL            EPSIL;
          BEGIN
REAL            KGO;
LABEL           AGAIN,EXIT,L9,SKIP,TEST;
OWN REAL ARRAY  C[0:N,0:N],          E[0:N,0:N];
COMMENT         C = A × B;
TEST;           FOR I ←1, I+1 STEP 1 UNTIL N DO BEGIN
                FOR J ←1, J+1 STEP 1 UNTIL N DO BEGIN
                C[I,J] ← 0.0;
                FOR K ← 1, K+1 STEP 1 UNTIL N DO BEGIN
                C[I,J] ← C[I,J] + A[I,K] × B[K,J]; END;
                END;
```

```
                    END;
COMMENT             TEST FOR ACCURACY;
                    FOR I ←1, I+1 STEP 1 UNTIL N DO BEGIN
                    J ← I;
                    IF ABS(C[I,J]-1.0) > EPSIL THEN GO TO AGAIN;
                    END;
COMMENT             MAIN DIAGONAL PASSES ACCURACY TEST,TRY ZERO ELEMENTS;
L9:                 FOR I ← 1, I+1 STEP 1 UNTIL N DO BEGIN
                    FOR J ← 1, J+1 STEP 1 UNTIL N DO BEGIN
                    IF J = I THEN GO TO SKIP;
                    IF ABS(C[I,J]-0.0) > EPSIL THEN GO TO AGAIN;
SKIP:               END;
               END;
                    KGO ← 1.0;
COMMENT             D = 2I - C;
AGAIN:              FOR I ←1,I+1 STEP 1 UNTIL N DO BEGIN
                    FOR J ←1,J+1 STEP 1 UNTIL N DO
                    D[I,J] ← -C[I,J];
                    END;
                    FOR I ←1,I+1 STEP 1 UNTIL N DO BEGIN
                    J ← I;
                    D[I,J] ← 2.0 - C[I,J];
                    END;
                    IF KGO = 1.0 THEN GO TO EXIT;
COMMENT             B = B×D;
                    FOR I ← 1, I+1 STEP 1 UNTIL N DO BEGIN
                    FOR J ← 1, J+1 STEP 1 UNTIL N DO BEGIN
                    E[I,J] ← 0.0;
                    FOR K ←1, K+1 STEP 1 UNTIL N DO BEGIN
                    E[I,J] ←  E[I,J] + B[I,K] × D[K,J];END;
                    END;
                    END;
                    FOR I ←1,I+1 STEP 1 UNTIL N DO BEGIN
                    FOR J ←1,J+1 STEP 1 UNTIL N DO BEGIN
                    B[I,J] ←  E[I,J]; END;
                    END;
```

```
                    GO TO TEST;
EXIT:               END;
                    FOR I ←1,I+1 STEP 1 UNTIL 4 DO BEGIN
                    READ(CARD,FIN,L1); END;
                    FOR I← 1,I+1 STEP 1 UNTIL 4 DO BEGIN
                    READ(CARD,FIN,L2); END;
                    MATRIT(4,A,B,0.01);
                    FOR I ←1, I+1 STEP 1 UNTIL 4 DO BEGIN
                    WRITE(LINE,FOT,L2); END;
                    WRITE(LINE,FOT2);
                    FOR I ←1, I+1 STEP 1 UNTIL 4 DO BEGIN
                    WRITE(LINE,FOT,L3); END;
               END.
```

Appendix A - Matrix Iteration

None of the inversion methods presented in this report can guarantee predicted accuracy, although they may be extremely accurate in some cases. A subroutine or procedure for improving the accuracy of an approximate solution (using the method described in Reference 3) has therefore been written in Algol and is included here.

MATRIT

Suppose that a matrix [B] has been obtained that is very nearly equal to $[A]^{-1}$. We can then write

$$[B] + [\epsilon] = [A]^{-1} \tag{1}$$

$$[A]([B] + [\epsilon]) = [I]$$

$$[A] \cdot [\epsilon] = [I] - [A] \cdot [B]$$

$$[B] \cdot [A] \cdot [\epsilon] = [B]([I] - [A] \cdot [B])$$

Since $[B] \cdot [A]$ is approximately $[A]^{-1} \cdot [A] = [I]$

$$[\epsilon] \approx [B]([I] - [A] \cdot [B])$$

From (1) $$[A]^{-1} \approx [B] + [B]([I] - [A] \cdot [B])$$

Using this formula for an iteration process we can write

$$[B_2] = [B_1](2[I] - [A] \cdot [B_1])$$

Until $[B_n] + [\epsilon] = [A]^{-1}$ and ϵ can be made as small as is desired.

A procedure to perform this iteration follows. The program listing includes a sample driver program for a 4×4 matrix which was checked with a hand calculation. The procedure is entitled MATRIT and can be called upon after the compilation of any inversion program to iterate to as high a degree of accuracy as is desired by proper selection of the input variable EPSIL. The output of this program gives the inverted matrix after accuracy requirements have been met and prints out the product of the original and inverted matrices so that accuracy can be checked by inspection. One caution when using this procedure: no test has been incorporated to determine if convergence can be expected. Since the time for machine calculation for matrix multiplication is quite lengthy (about 4 minutes for a 90×90 matrix multiplied

with its inverse) and since 2 multiplications are required for each iteration, the procedure should be monitored carefully until a convergence test and a "maximum number of iterations" option are included.

Appendix B - Inversion of a Matrix by Partitioning

It is sometimes more efficient to deal with portions of a matrix rather than the entire array. For extremely large matrices this may be the only way to invert the matrix.

A scheme is given here for subdividing or partitioning an $n \times n$ matrix [S] into four parts.

Let

$$[S] = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

where [A] and [D] are square non-singular matrices of order p and q respectively; the inverse of [S], $[S]^{-1}$ can be written

$$[S]^{-1} \begin{bmatrix} K & L \\ M & N \end{bmatrix}$$

Expressions for solving for K L M and N are derived here. In conformity with the rule for multiplying partitioned matrices, the following matrix equations hold.

$$[S] \cdot [S]^{-1} = [I]$$

$$\begin{bmatrix} [A] & [B] \\ [C] & [D] \end{bmatrix} \cdot \begin{bmatrix} [K] & [L] \\ [M] & [N] \end{bmatrix} = \begin{bmatrix} I & O \\ O & I \end{bmatrix}$$

omitting brackets

$$A \cdot K + B \cdot M = I \qquad (1)$$
$$A \cdot L + B \cdot N = O \qquad (2)$$
$$C \cdot K + D \cdot M = O \qquad (3)$$
$$C \cdot L + D \cdot N = I \qquad (4)$$

Multiplying (3) by $B \cdot D^{-1}$ and subtracting from eq (1)

$$(A - B \cdot D^{-1} \cdot C) K = I$$

therefore: $K = (A - B \cdot D^{-1} \cdot C)^{-1}$

Similarly $N = (D - C \cdot A^{-1} \cdot B)^{-1}$

From (3) $M = - D^{-1} \cdot C \cdot K$

and from (2) $L = - A^{-1} \cdot B \cdot N$

However, this involves four inversions. Therefore these results are expressed in an alternate form

$$N = (D - C \cdot A^{-1} \cdot B)^{-1}$$

$$M = - N \cdot C \cdot A^{-1}$$

$$L = - A^{-1} \cdot B \cdot N$$

$$K = A^{-1} - A^{-1} \cdot B \cdot M$$

or, if it appears that the matrix D will invert more easily than A, use

$$N = D^{-1} - D^{-1} \cdot C \cdot L$$

$$M = - D^{-1} \cdot C \cdot K$$

$$L = K \cdot B \cdot D^{-1}$$

$$K = (A - B \cdot D^{-1} \cdot C)^{-1}$$

reducing the number of inversions to two. Procedures for inversion and matrix multiply are available and matrix subtraction implies that the matrices are conformable (of the same order) and element by element subtraction performs this operation.

Rules for partitioning a matrix into nine parts did not appear to be available in the literature and were developed here by similar manipulations.

For a matrix [M] where

$$[M] = \begin{bmatrix} A & B & C \\ D & E & F \\ G & H & Z \end{bmatrix} \qquad [M]^{-1} = \begin{bmatrix} P & Q & R \\ S & T & U \\ V & W & X \end{bmatrix}$$

where

$$P = A^{-1}[I - (BS + CV)]$$

$$Q = - A^{-1}(BT + CW)$$

$$R = - A^{-1}(BU + CX)$$

$$S = (E - DA^{-1}B)^{-1}[(DA^{-1}C - F)V - DA^{-1}]$$

$$T = (E - DA^{-1}B)^{-1}[I + (DA^{-1}C - F)W]$$

$$U = (E - DA^{-1}B)^{-1}[DA^{-1}C - F]X$$

$$V = [(Z - GA^{-1}C) + (H - GA^{-1}B)(E - DA^{-1}B)^{-1}$$
$$(DA^{-1}C - F)]^{-1}[(H - GA^{-1}B)(E - DA^{-1}B)^{-1}DA^{-1} - GA^{-1}]$$

$$W = X[-(H - GA^{-1}B)(E - DA^{-1}B)^{-1}]$$

$$X = [(Z - GA^{-1}C) + (H - GA^{-1}B)(E - DA^{-1}B)^{-1}(DA^{-1}C - F)]^{-1}$$

Appendix C - Selected Outside Programs

There are several programs in the Denver area which are capable of performing operations with larger matrices than we can successfully operate on here. These programs are available at the Martin Company and at the National Bureau of Standards. Purchase order contracts are necessary to obtain machine time with both agencies and the cost in both cases is quite high. Each of the three programs briefly described here uses either auxiliary tape units (PN LAMI, JD020), computes with double precision arithmetic (PN LAMI) or is a special purpose routine (JD041).

A. F1 PN LAMI 3011 (Bureau of Standards)

Research Institute of National Defense - Sweden Large Matrix Inversion and Solution of Linear Equations, Fortran - FAP routine (double precision).

The Fortran - FAP routine solves the matrix equation $[A]\{X\} = \{B\}$. $[A]^{-1}$ is also obtained, in fact inversion may be the sole aim.

1. Mathematical Theory

Jordan's method is used to reduce a matrix [A] to the Identity matrix through a succession of elementary eliminations. These transformations are simultaneously applied to the identity matrix and adjoined matrix [B] which results in the inverted matrix $[A]^{-1}$.

2. Accuracy and Machine Time

The accuracy obtained depends, of course, upon the condition of the input matrix. A test run with a matrix of order 200 where all the coefficients were random numbers uniformly distributed between -10 and +10 showed a maximum error of 0.23×10^{-12}. Machine time for the inversion was just over one hour which is very nearly equal to the estimated time for inversion given in the program write-up as $(0.288N + 29.0)\ N^2$ ms.

B. J0041 Eigenvalue - Eigenvector Determination (Martin Company)

This Fortran - Machine Language program accepts manipulated input data in such a manner that unrestrained structural vibration

problems can be solved accurately in the low frequency range by circumventing problems associated with numerical round-off. Essentially, the program solves a set of homogeneous second order differential equations of the form

$$[M]\{\ddot{X}\} + [K]\{X\} = 0$$

where [M] is the symmetric mass matrix and [K] is a symmetric stiffness matrix. The program solves for the eigenvalues $[\mu]_i$ and $[\phi_{\mu i}]$, the matrix of vectors of the system.

1. Machine Time and Accuracy

The total time for computation and printout for each consecutive run is determined by the size and density of the input matrices. Approximately five minutes were required for one run of a matrix 60 × 60. Additional time must be allowed for a high degree of accuracy. Accuracy is determined by an input variable FT. As FT becomes smaller the accuracy for this iterative method increases as does the machine time.

It can be shown that the eigenvalues $\mu_j = \frac{1}{\omega_j^2}$, where ω_j^2 equals the circular frequency squared. The accuracy of the highest μ's (and therefore the lowest ω's) can be computed to a very high degree of accuracy; however the accuracy of the lowest valued μ's is not adequate for many applications, particularly if there are several zero valued roots, making the program excellent for solving vibration problems for the low frequency range.

C. JD020 Solution of Simultaneous Equations, Fortran-Machine Language (Martin Company)

This method for finding a matrix inverse by solving the set of equations

$$[A]\{X\} = \{I_j\}$$

where $\{I_j\}$ is input column by column as the Identity matrix of consecutive right hand sides, has proven to be a highly successful method. The program does not require that the coefficient matrix A must be symmetrical. Unless programming modification is available each non-zero element must be input for the entire matrix. Acceptable accuracy has

been obtained by users for matrices up to 300 × 300. Matrix multiplication is the only method for ascertaining accuracy. Multiplications use a great deal of machine time (at purchase rates) and it may be that several typical rows and columns can be sampled for accuracy.

FINAL REPORT

FEASIBILITY OF X-RAY STUDIES OF LIQUID METALS

M. J. Pool

Project 623

Attention: Chairman, Awards Committee
Professor S. A. Johnson, Jr.

Metallurgy Division
Denver Research Institute
University of Denver

September 1965

APPROVED BY:

Charles E. Lundin
Acting Division Head

PREPARED BY:

Monte J. Pool
Research Metallurgist

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ABSTRACT

Visits were made to the University of Arkansas, University of Missouri and Massachusetts Institute of Technology to discuss the feasibility of using X-ray diffraction techniques to study the structure of dilute liquid metallic solutions.

The principal people visited were Drs. R. F. Kruh, G. T. Clayton, N. S. Gingrich, C. W. Tompson and R. Kaplow.

I. INTRODUCTION

In order to determine the feasibility of studying dilute solutions of liquid tin alloys by X-ray diffraction techniques travel funds were provided under NASA grant NsG-518. These funds were used to visit several outstanding people in the field of study of liquid structures by X-ray diffraction techniques. The people visited were Dr. R. F. Kruh and Dr. G. T. Clayton of the University of Arkansas, Dr. N. S. Gingrich and Dr. C. W. Tompson of the University of Missouri and Dr. Roy Kaplow of the Massachusetts Institute of Technology. Discussions were also held with several graduate students currently working in the field of liquid structures at these institutions.

II. RESULTS OF VISITS

The discussion sessions centered around experimental techniques, equipment design and data analysis. Every facility visited is currently using a θ-θ diffractometer for the study of liquid structures. This arrangement maintains a stationary sample with the X-ray source and detector unit rotating together, thus maintaining the necessary 2θ relationship between the incident and reflected beams. Monochromatization is accomplished by using a LiF or NaCl monochromator. This is placed either between the source and the sample or between the sample and the detector. Both techniques are currently being used and one does not have any appreciable advantage over the other.

Both proportional counters and scintillation counters with discriminators are being used to monitor the intensity of the diffracted beam. In general it is felt that the proportional counter is superior. Step scanning is also used with a constant counting time.

The most important phase of the discussions was concerned with data analysis. This consisted mainly of discussing methods to eliminate errors in the radial distribution function, which is obtained by Fourier inversion of the intensity data. A number of points were discussed along these lines and these are summarized below.

(1) The correct absorption coefficient must be used.
(2) The fitting process must be exact and free of termination errors.
(3) Second order half-wavelength reflections must be eliminated.
(4) X-ray flourescence from the sample must be avoided.
(5) The coherent and incoherent contributions must be precisely known.

III. CONCLUSIONS

Even though no work has been done in the past on X-ray studies of very dilute liquid solutions, the consensus of opinion was that significant results could be obtained by using this technique. It would be necessary to use a θ-θ diffractometer and exercise extreme care in the data analysis. As a result of these discussions a proposal will be submitted to the NASA Awards Committee requesting funds for the purchase of a θ-θ diffractometer. The estimated cost of this equipment is $30,000.

IV. ACKNOWLEDGEMENT

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